

**U. S. DEPARTMENT OF THE INTERIOR  
GEOLOGICAL SURVEY**

**PROPERTIES AND HAZARDS OF  
108 SELECTED SUBSTANCES - 1990 EDITION**

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NOTICE

The information in this document has been funded in part by the United States Environmental Protection Agency under interagency agreement DW14932497-01-1/2 to the United States Geological Survey. It has been subjected to Agency review and approved for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

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## INTRODUCTION TO OPEN-FILE REPORT 89-491

The Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), commonly known as Superfund, was passed into law in December 1980. The Superfund Amendments and Reauthorization Act (SARA) was signed into law on October 17, 1986. The Superfund program identifies hazardous waste sites, evaluates waste damage to natural resources, ensures a clean up by responsible parties or government, and establishes a claims procedure for costs or damages. Superfund regulations affect past actions rather than ongoing activities.

The Resource Conservation and Recovery Act (RCRA) was enacted as Public Law 94-580 in 1976. RCRA was amended by the Used Oil Recovery Act of 1980 and the Hazardous Solid Waste Amendments of 1984. The primary goal of RCRA is to protect human health and the environment. It is RCRA that provides for the "cradle to grave" management of hazardous waste, from generator to transporter to storage or disposal.

The establishment of the Superfund and RCRA programs reflects our society's great use of hazardous substances and, at the same time, our increased concern for health and environmental dangers these substances present. To protect the quality of the air we breath, the environment we work in, and water we drink, the Clean Air Act was passed in 1955, the Occupational Safety and Health Act in 1970, and the Safe Drinking Water Act Amendments in 1986. The Environmental Protection Agency (EPA) is the primary government agency authorized to develop regulations to carry out and enforce the statutes in all five of these programs. In response, the EPA has developed the first priority list of over 100 of the most hazardous substances, standards for control of air pollution, and regulations and guidelines for the presence of drinking water contaminants.

This report summarizes information on physical, chemical and thermodynamic properties, uses, fire and explosion hazards, handling precautions, health hazards, and toxicity for 107 hazardous substances and water. Twenty of these are some of the most commonly occurring organic ground water contaminants found at hazardous waste disposal sites (Plumb and Pitchford 1985). Ninety-eight substances are on the U.S. Environmental Protection Agency "top 100" hazardous substances list. Forty-six are regulated drinking water contaminants. The 107 substances are mostly organic chemicals, but there are a few inorganic chemicals and some elements.

The EPA top 100 list actually contains more than 100 substances because many are grouped together (see Table 1). Nineteen substances on the list are left out of this report because of lack of data (see Table 15). Some of the top 100 substances, such as cyanide, are included as their most commonly occurring compounds. Other substances on the list, such as total xylenes, are represented by the individual isomers. In the case of the seven PCBs on the list, only one is represented here.

The Chemical Abstracts Service Registry Number (CAS RN) is provided as an identifier of each substance. The substances in this report appear in alphabetic sequence and generally are named using nomenclature standards established in the Chemical Abstracts Service Registry Handbook (American

Chemical Society 1980). A few are listed using their more familiar names (such as DDT). Water is included for reference and as a standard for calibration and comparison.

The data were compiled from handbooks, texts, and reports listed in the annotated reference, the electrochemical data reference, and the clay-organic interaction reference sections. Annotated references are noted in brackets following the numeric data and information for each substance. Rather than selecting what we thought was the best property value for a substance, we included all the values found and let the reader decide the most reasonable. Values that were obvious typographical errors were not included. In almost all cases, the cited references are not the primary investigators. The quoted sources should be examined for the original reference. Though thirty-two references were used as sources for the property data, Sax 1984 [51], Dean 1985 [10], Weast 1988 [105], Riddick et al. 1986 [49], and Weiss 1986 [107] accounted for about 55% of the data. Another 26% of the information was taken from Hawley 1981 [22], Mackison et al. 1981 [32], Verschueren 1983 [104], Windholz 1983 [108], and Sittig 1985 [56]. The remaining 19% of the data was taken from the other references.

Care was taken to include all available data in an accurate and concise format. The chemical and physical property values are quoted from the noted references. The order of reference numbers generally reflects the order in which they were referred to and not meant to suggest one as more significant than another. Definitions for all properties and conversion factors are discussed in "The Properties" section of this report. Synonyms, including registered and unregistered trade names and common and generic terms that have been accurately or ambiguously applied to these substances, are supplied in Table 3 and for each substance. It is noted that some synonyms were incorrectly applied in the literature but are included here because of former usage. Molecular formulas are given and the structural formula in the cases of complex molecules. Fire and explosion hazards are briefly summarized in terms of explosive limits, flash points, extinguishing agents, and incompatible materials. The various uses of the substances are noted as well.

The health and toxicity data represent observed as well as speculated effects on humans. The primary references for this information were Strauss and Kaufman 1976 [57], Mackison et al. 1981 [32], Verschueren 1983 [104], Sax 1984 [51] and material safety data sheets (MSDS), especially the Sigma-Aldrich MSDS (Sigma-Aldrich Corp. 1989 [55]). Detailed discussions of the toxicity of the elements and inorganic compounds are contained in Seiler and Sigel 1988 [54]. The procedures and information in this report reflect safe laboratory practices and the availability of health hazard studies, but are presented in summary form. The references and the original RTECS entries should be consulted for more complete information and to assure compliance with safety regulations. It is the user's responsibility to determine the suitability of this information for the adoption of appropriate safety precautions. Appropriate manuals (such as Mackison, et al. 1981 [32], Bretherick 1981, and material safety data sheets) should be referred to for first aid procedures. All substances should be disposed of in accordance with all applicable federal, state and local environmental regulations. Contact local, state, and federal health and waste management and regulatory agencies for proper and legal disposal

and waste management and regulatory agencies for proper and legal disposal and handling procedures.

Tables that summarize and compare various properties of the substances appear near the beginning of the report. These tables allow the reader to find a substance based on the CAS RN, chemical formula, or by synonym. An additional table is included discussing the maximum contaminant levels and guidelines established by the EPA for drinking water contaminants. The references, a brief bibliography, and a cross-reference table, or index of synonyms, conclude the report.

The data and information compiled in this report represent a portion of the Toxic Waste Geophysics investigations being conducted by the U.S. Geological Survey, [Branch of Geophysics]. This report is an expanded and revised version of the USGS Open-File Report 87-428 (Lucius 1987). The authors are not aware of any other single document that presents such a comprehensive list of properties for the selected substances as this one does. Much of the data will be condensed into the data base for the next revision of the current USGS Geophysics Advisor Expert System (Olhoeft 1988) available on flexible diskette.

One purpose in compiling this report is to define data "gaps" concerning physical and chemical properties, electrochemical properties and clay-organic interactions of these substances. As missing data for these and other properties are gathered, the report will be updated. References for electrochemical properties and clay-organic interactions reflect only an initial search of the literature. More thorough literature searches are planned before the next update is published. Only references are noted for the electrochemical data. For clay-organic interactions, topics rather than data are summarized from some of the cited references.

This report is intended to be used principally by the laboratory investigator. However, it also may be useful to field engineers, scientists and others involved with hazardous waste management and investigations. It may be particularly useful to those assigned the responsibility of rating hazard potential of waste disposal facilities. The EPA has adopted a system for rating hazard potential of waste disposal facilities which includes assessing waste characteristics (Kufs et al. 1980). The rating factors for determining waste characteristics are toxicity, radioactivity, persistence, ignitability, reactivity, corrosiveness, solubility, volatility, and physical state. All of these factors (and many more) are discussed in this report, excluding radioactivity.

The authors encourage readers to contribute new data concerning these substances and to correct any errors.

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## INTRODUCTION TO 1990 EDITION

This report is a revised and updated version of the U.S. Geological Survey Open-File Report 89-491. The format has remained unchanged except for the addition of Henry's law constant in the analytical chemistry section. In addition, an extended literature search, particularly by Pat Hill, provided previously missing data values. Recent laboratory work by Edgar Ethington [18] provided contact angle measurements, which have not been available. A summary of this work is presented here (see Figures 1-4). Many typographic errors were also corrected and the definitions list has been expanded as well as the synonym, reference, and bibliography sections.

This report compiled data from 110 sources (versus 32 for the 1989 report) as source material for physical and chemical properties (many more were used to gather clay-organic interaction and electrochemical data). The 78 new references contributed about 9.5% of the approximately 13,175 occurrences of annotated references. Sax 1984 [51], Dean 1985 [10], Weast 1988 [105], Riddick et al. 1986 [49], and Weiss 1986 [107] still account for over 50% of the data.

The following discussion is in response to comments and questions concerning the 1989 report. This document was prepared using Microsoft Word 5.0 on an IBM compatible computer and printed using a variety of fonts on a HP LaserJet Series II. There are over 1.1 million characters in the document. Because of the large file size and MS Word formatting, we are not distributing this report on flexible diskettes. Most of the data will be incorporated into the second version of the Geophysics Expert Advisor System by Gary Olhoeft. This Open-File Report may be freely copied and distributed. Much of the data presented here was copied directly from the noted references. Only the most blatant errors were corrected. The quoted source should be examined to determine accuracy of the data and for more complete discussions of data acquisition and meaning. We include here most values for a particular property of a substance, so that the reader can determine the reliability and certainty of the data. In the sections on toxic exposure, "adult human", "child", or "infant" means gender was not specified in the reference. Often, there was a distinction made between adult males and adult females. The reader should consult the original reports for more detail.

The authors welcome all comments, particularly those concerning missing or inaccurate data.

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## THE PROPERTIES

This section contains brief discussions of the physical and chemical properties and chemical designations used in this report. A list of abbreviations and a conversion table for SI to cgs or English systems are also included. Property values are reported in SI units. An exception is temperature which is referred to in degrees Celsius (rather than Kelvin). Definitions were compiled from various sources in the reference and bibliography sections.

### Definitions

Autoignition temperature. The minimum temperature at which a substance can ignite or combust in the absence of a flame or spark. Also referred to as autoignition point or ignition point. Given in degrees Celsius at atmospheric pressure, unless stated otherwise.

Boiling point. The temperature at which the vapor pressure of a liquid is equal to or slightly greater than atmospheric pressure. Standard values are measured at one atmosphere and in degrees Celsius. Non-standard pressures are noted.

CAS Registry Number (CAS RN). A unique identifier assigned by the American Chemical Society to chemicals recorded in the Chemical Abstracts Service Registry System. This number can be used to access many chemical databases and to conclusively identify a substance regardless of name.

Ceiling limit (CL). American Conference of Governmental Industrial Hygienists (ACGIH) Threshold Limit Value (TLV). The ceiling limit is a concentration of a substance in air which can not be safely exceeded, even instantaneously.

Compressibility. The change in liquid density with pressure, measured as the ratio of volume change per unit change in pressure at a specified pressure (in this report, approximately one atmosphere). Units are reciprocal Pascals ( $\text{Pa}^{-1}$ ).

Contact angle. The angle (in degrees) a liquid drop of a substance makes on a specified substrate. The angle is measured through the liquid to a line tangent to the edge of the drop making contact with the substrate. Only four substrates are reported: quartz, calcite, biotite, and Ca-montmorillonite. Contact angle can be reported in three ways: sessile, advancing, and receding. The sessile contact angle is for a stable, non-moving drop on a smooth, flat, level substrate. For drops of liquid that are expanding, the advancing angle is measured at the moving, leading edge. The receding angle is measured for a contracting drop at the trailing edge. The larger the angle (in degrees), the more spherical the shape of the drop, and the more phobic the substance is to that substrate (i.e. non-wetting). See [18] for more complete discussion of the measurements, procedures, and uses.

Critical pressure. The lowest pressure (in megapascals, MPa) which will liquefy a vapor phase at its critical temperature. Above the critical pressure the liquid and vapor phases are no longer distinguishable.

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Critical temperature. The temperature (in degrees Celsius) above which the vapor phase cannot be condensed by an increase in pressure.

Dielectric constant. See relative dielectric permittivity.

DOT Designation. A four digit number assigned by the U.S. Department of Transportation for hazardous materials and is identical to the United Nations identification number (which is preceded by the letters UN). This number is required on shipping papers, placards, and labels. DOT numbers, if available, can be found in the synonym lists.

Dynamic viscosity. The ratio between the applied shear stress and the rate of shear. The force per unit area necessary to maintain a unit velocity gradient at right angles to the direction of flow between two parallel planes a unit distance apart. Also called coefficient of viscosity. Given in millipascal-seconds,  $10^{-3}$  Pa-s (mPa-s).

Electric dipole moment. The distance (in meters) between charges multiplied by the quantity (magnitude) of electric charge (in coulombs). Occurs in molecules in which the atoms and their electrons and nuclei are so arranged that one part of the molecule has a positive charge while the other part is negatively charged. Given here for the gas phase of the substance in coulomb-meters (C-m).

Electrical resistivity. The amount of electrical potential loss (in volts per ampere, or ohms) during unit time between unit areas separated by unit distance. Values given here are in megohm-meters squared per meter simplified to megohm-meters (MOhm-m) for current flow in the pure liquid or solid phase of the substances. The reciprocal of resistivity is conductivity.

Evaporation rate. The ratio of the time of evaporation of a specific amount of a substance compared to the evaporation time of the same amount of butyl acetate. A relative value where butyl acetate has a value of 1.

Explosive limits. The range of concentrations of a flammable gas or vapor (percent by volume in air) in which an explosion can occur upon ignition in a confined area.

Flash point. The minimum temperature (in degrees Celsius) at which the vapor pressure above a liquid or solid is high enough to result in ignition. Substances with flashpoints  $<100^{\circ}\text{C}$  can be considered dangerous. Testing methods noted, if reported in the literature, are open Cleveland cup (OC) (ASTM method D93) and Tag closed cup (CC) (ASTM method D56). The open cup method is more representative of natural conditions.

Gibbs (free) energy. The maximum useful work that can be obtained from a chemical system without net change in temperature or pressure. Under conditions of constant pressure and temperature, a process can only occur in the direction of decreasing Gibbs (free) energy. Given in kilojoules per mole (kJ/mol) at the specified temperature.

Heat. A mode of energy associated with and proportional to molecular motion. It can be transferred from one body to another by radiation, convection or conduction.

Heat capacity. The quantity of heat required to raise a liquid chemical system one degree in temperature, at 25°C or as noted and constant pressure. Given in kilojoules per mol-degree Kelvin (kJ/(mol-K)).

Heat of combustion. The amount of heat released in the oxidation (burning) of one mole of a substance at a constant pressure or constant volume. A negative value indicates heat is given off. Given in kilojoules per mole (kJ/mol) at the specified temperature.

Heat of formation. The heat evolved or absorbed when a compound is formed in its standard state from elements in their standard state at 25°C and one atmosphere. A negative value indicates heat is given off. Given in kilojoules per mol (kJ/mol).

Heat of melting. The heat required to convert one mole of a substance from solid to the liquid state with no temperature change. Also referred to as heat of fusion. Given in kilojoules per mole (kJ/mol).

Heat of sublimation. The heat required to convert one mole of a solid to a vapor at constant pressure and temperature without the appearance of liquid. Given in kilojoules per mole (kJ/mol).

Heat of vaporization. The heat required to convert one mole of a liquid to the gaseous phase with no temperature change. Given in kilojoules per mole (kJ/mol) at the boiling point of the liquid or as specified.

Henry's law constant (H). The air/water partition coefficient. It relates the substance (solute) concentration in the gas phase to its concentration in the water phase. In other words, it is the ratio of the partial pressure of a substance in air to the concentration of the substance in water at a given temperature under equilibrium conditions. A non-dimensional H can be calculated using the following formula,

$$H = \frac{S_a}{S_w}$$

where

H = dimensionless Henry's law constant  
 $S_a$  = solute concentration in air (mol/L)  
 $S_w$  = aqueous solute concentration (mol/L).

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Alternatively, a dimensional H can be calculated using,

$$H' = \frac{P \times FW}{S}$$

where

H' = Henry's law constant (kPa-m<sup>3</sup>/mol)  
P = vapor pressure (kPa)  
FW = relative molecular mass (g/mol)  
S = solubility (mg/L)

H is a useful parameter for quantifying the potential for volatilization of dissolved compounds. Both dimensional and dimensionless values are reported.

Hydrolysis half-life. The time (in seconds) for half of the concentration of organic chemical in water to undergo a hydrolysis reaction (see Dragun 1988 [13]). Hydrolysis is a chemical reaction in which water reacts with another substance to form two or more new substances and ionization of the water molecule.

IDLH value. The Immediately Dangerous to Life and Health exposure concentration guidelines developed by NIOSH and OSHA. They represent a maximum concentration (in ppm) from which a person could escape within thirty minutes without any impairing symptoms or irreversible health effects.

Ionization potential. The minimum energy required to remove the least strongly bound electron from a molecule to form a positive ion. Given in electron volts (eV). Symbols for some principal methods are:

EI - electron impact  
PE - photoelectron spectroscopy  
PI - photoionization  
S - optical spectroscopy  
VUS - vacuum ultraviolet spectroscopy.

Kinematic viscosity. The ratio of the dynamic viscosity to the density of a fluid. Given in micrometers squared per second, 10<sup>-6</sup> m<sup>2</sup>/s (μm<sup>2</sup>/s). Calculated from the dynamic viscosity and specific gravity. These values are approximate as the density varies slightly with temperature.

Lower explosion limit (lel). The minimum volume percent of a substance in air which can be ignited.

Loss tangent. The dielectric loss tangent. The ratio of imaginary to the real portions of the complex permittivity. It is a measure of the dielectric loss, i.e. the energy loss per cycle in a dielectric material due to conduction and slow polarization currents or other dissipative effects. Also referred to as the dielectric dissipation factor.



Magnetic volume susceptibility. The ratio of the intrinsic induction due to the magnetization of a material to the induction in vacuum due to the influence of the corresponding magnetizing force. A dimensionless quantity. All the substances in this report with values listed are called diamagnetic, that is, their magnetic susceptibilities are very slightly negative.

Melting point. The temperature (in degrees Celsius) at which the liquid and crystalline phase of a substance are in equilibrium, usually measured at one atmosphere. The term is often used interchangeably with freezing point.

Molarity. A one molar concentration (M) equals one mole of a substance dissolved in one liter of solution.

Molecular formula. A non-graphic representation of atoms or group(s) of atoms relative to each other.

Mole (mol). The amount of pure substance containing Avogadro's number of atoms or molecules (i.e.,  $6.022045 \times 10^{23}$ ). It is the number of atoms in exactly 12 grams of carbon-12. For example, 10 grams of  $H_2O$  will contain  $10.0/18.0152$  moles of  $H_2O = 0.5551$  mol, where 18.0152 is the relative molecular mass of  $H_2O$ .

Partition coefficient (pP<sub>oct</sub>). A measure of the distribution of a given compound (solute) in two phases and expressed as a concentration ratio, assuming no interactions other than simple dissolution. It is the ratio of the equilibrium concentration  $C$  of a dissolved substance in a two-phase system consisting of two generally immiscible solvents, in this case  $n$ -octanol and water. Partition coefficients are valuable in describing the environmental behavior of compounds in terms of soil or sediment adsorption and biological uptake, and can be related to molecular surface area and molar refractions. It is usually given as the logarithm (to base 10) of the ratio.

$$pP_{oct} = \log_{10} \left[ \frac{C_{octanol}}{C_{water}} \right]$$

pH. A value taken to represent the acidity or alkalinity of an aqueous solution. It is defined as the negative logarithm (to base 10) of the hydrogen ion concentration of a solution.  $pH = -\log_{10}[H^+]$ . For example, pure water dissociates to  $H^+$  and  $OH^-$  with a concentration  $[H^+] = 1 \times 10^{-7}$  parts to one part water, a pH of 7.

pK. A measure of the completeness of an incomplete chemical reaction. Defined as the negative logarithm (to base 10) of the equilibrium constant,  $K$ , for the reaction in question.  $pK = -\log K$ .  $K$  is defined for the reaction  $aA + bB \rightarrow cC + dD$  as:

$$K = \frac{[C]^c \times [D]^d}{[A]^a \times [B]^b}$$

## 10 - Properties

**pK<sub>a</sub>.** The negative log (to base 10) of the acid dissociation constant which is

$$K_a = \frac{[H^+][A^-]}{[HA]}$$

where [] indicates molar concentration (for dilute solutions).

pK<sub>a</sub> = -log<sub>10</sub>K<sub>a</sub>. It expresses the extent of dissociation, or the strength, of weak acids. The smaller the pK<sub>a</sub>, the more readily the acid dissociates (i.e., the stronger the acid). Strong acids will have values <5, and weak acids will have values >5 for their pK<sub>a</sub>. In a solution of a weak acid, if the concentration of undissociated acid is equal to the concentration of the anion of the acid, the pK will be equal to the pH. The degree of dissociation affects processes such as photolysis, protolysis, evaporation from water, soil or sediment absorption, and bioconcentration.

**pK<sub>BH</sub>.** The negative log (to base 10) of the ionization constant of a protonated base.

**pK<sub>s</sub>.** The negative log (to base 10) of the autoprotolysis constant of a solvent employed in nonaqueous acid-base titrations in 0.01M solution.

**pK<sub>w</sub>.** The negative log (to base 10) of the ionization constant of water.

**Refractive index.** The dimensionless ratio of the velocity of light (normally using the yellow D line of the sodium spectrum, 589.6 nm) in air to its velocity in the substance. Measured at 20°C, or as noted.

**Relative dielectric permittivity.** The dielectric permittivity of a substance relative to that of vacuum (formerly called dielectric constant). The real part of the relative complex permittivity. It is a measure of the capacity of a material to store charge when an electric field is applied. The relative dielectric permittivity is temperature and frequency dependent and these values are noted if cited in the literature.

**Relative molecular mass.** The sum of the relative atomic masses (formerly atomic weights) of the elements in a molecule. Formerly referred to as molecular weight. Molecular mass is a fundamental characteristic of a chemical compound and can be used to estimate other properties. The calculation of relative molecular masses was made using the following values from [105].

Bromine	= 79.904
Carbon	= 12.011
Chlorine	= 35.453
Fluorine	= 18.9984
Hydrogen	= 1.00794
Nitrogen	= 14.0067
Oxygen	= 15.9994
Potassium	= 39.0983
Sodium	= 22.9898
Sulfur	= 32.06

Relaxation time. The dielectric relaxation time constant. The reciprocal of the preferred frequency at which maximum dampening of polarization processes in materials occurs. The time (in seconds, s) for a current to decay to  $1/e \approx 0.368$  of its value after the electromagnetic field is removed.

Short Term Exposure Limit (STEL). ACGIH TLV value. The STEL is a 15-minute time-weighted average exposure concentration (in ppm) which should not be exceeded any time during an eight hour work day. Excursions to the STEL level should be separated by one hour, should not be longer than fifteen minutes in duration, and should not be repeated more than four times a day.

Solubility. The ability of a substance to be dissolved in various solvents. It can be described as follows using weight percentages (wt%):

miscible	(dissolves 100%)
very soluble	(>50%)
soluble	(5-50%)
slightly soluble	(<5%)
insoluble	(0% or <0.001%).

Water solubility provides insight into the fate and transport of a chemical in the environment. Besides determining whether a chemical will partition to water or partition to soil or sediment or bioconcentrate in aquatic organisms, solubility may also affect photolysis, hydrolysis, oxidation, and washout from the atmosphere by rain.

Solution diffusivity. The rate of diffusion of dilute solutions of the listed solute in various solvents at one atmospheric pressure, in nanometers squared per second,  $10^{-9} \text{ m}^2/\text{s}$  ( $\text{nm}^2/\text{s}$ ).

Specific gravity. The dimensionless ratio of the density of the substance, at 20°C, to the density of pure water at 4°C (actually 3.98°C), i.e. at 20/4, or at temperatures noted, and one atmosphere pressure. At 20/4, the specific gravity is equivalent to density.

Speed of sound. The speed of sound (compressional elastic) waves in the liquid substance. It is dependant on temperature, pressure and to some extent frequency. Measured in meters per second (m/s) at the specified temperature and one atmosphere. For the solid elements, the speed of sound is reported for longitudinal and shear waves in the bulk material or in thin rods.

Structural formula. A graphic representation of atoms or group(s) of atoms relative to each other.

Surface tension. The force per unit length on the surface that opposes the expansion of the surface. It may be noted whether the substance is in contact with air or vapor. Liquids with high surface tensions show less tendency to spread. Given in millinewtons per meter (mN/m).

## 12 - Properties

Synonyms (syn). Includes codes and common, trivial, and commercial names. Registered trademarks are generally not identified as such. Note: Some names may be ambiguously or incorrectly applied.

Thermal conductivity. The quantity of heat conducted per unit time through unit area of unit thickness of a material having unit temperature difference between its faces. The heat flow across a surface per unit area per unit time, divided by the negative of the rate of change of temperature with distance in a direction perpendicular to the surface. Given in watts per meter-degree Kelvin, W/(m-K).

Thermal expansion coefficient. The change in volume per unit volume of the liquid or solid substance per degree change in temperature. Given in reciprocal Kelvins ( $K^{-1}$ ).

Threshold Limit Value (TLV). Formerly known as Maximum Allowable Concentration (MAC). The threshold limit values refer to airborne concentrations of substances (in ppm or  $mg/m^3$ ) and represent a "threshold" dose below which there are no known adverse effects. These exposure guidelines are developed by the American Conference of Governmental Industrial Hygienists (ACGIH) annually. TLVs are differentiated into three values based on exposure and concentration: time-weighted average concentration (TWA), short term exposure limit (STEL), and ceiling limit (CL).

Time-Weighted Average (TWA). ACGIH TLV value. The average concentration (in ppm) most workers can be exposed to for eight hours per day, five days a week without showing any adverse effects. A caution against skin contact is noted by "(skin)".

Upper explosion limit (uel). The maximum volume percent of the substance in air which can be ignited. If exceeded, the mixture cannot be ignited and sustain combustion.

Vapor density. The dimensionless ratio of the density of a gas to the density of an equal volume of air. Vapors with densities  $>1$  will sink.

Vapor diffusivity. The rate of diffusion of the compound as a vapor in air, in micrometers squared per second,  $10^{-6} m^2/s$  ( $\mu m^2/s$ ).

Vapor pressure. The partial pressure (in kilopascal, kPa) exerted by the vapor of a solid or liquid when in equilibrium with the solid or liquid at the stated temperature. vapor pressure provides insight into the transport of a substance in the environment. It can indicate how quickly a substance will evaporate and thus is useful in evaluating spills.

## Abbreviations

A	ampere, base SI unit of electric current
ACGIH	American Conference of Governmental Industrial Hygienists
allow	allowable
ANSI	American National Standards Institute
aq	aqueous
atm	standard atmosphere, a unit of pressure
Autoign. temp.	autoignition temperature
b	bar, unit of pressure (of fluid)
bp	boiling point
BTU	British thermal unit
C	coulomb, s-A, SI unit of electric charge, electric flux and elementary charge
°C	degree Celsius, SI unit of Celsius temperature and temperature interval
cal	calorie, thermochemical; also called gram calorie
calc	calculated
Ca-mont.	Ca-montmorillonite (clay), see van Olphen and Fripiat (1979)
CAS RN	Chemical Abstracts Service Registry Number
(CC)	closed cup flash point tester, kind not specified
CL	OSHA ceiling limit for human exposure
C-m	coulomb-meter
cm	centimeter
cmpd, cmpds	compound, compounds
CNS	central nervous system
cP	centipoise
CPE	Chlorpel®, chlorinated polyethylene
cSt	centistoke
D	Debye unit of dipole moment
dm	decimeter
dyn	dyne, g-cm/s <sup>2</sup> , 10 <sup>-5</sup> N, cgs unit of force
est	estimate
eV	electron volt, unit of energy
(EI)	electron impact method to measure ionization potential
°F	degree Fahrenheit, unit of Fahrenheit temperature and temperature interval
fp	freezing point
ft	foot
ft-lbf	foot pound-force
g	gram
µg	microgram
(gas)	gaseous or vapor phase
Hg	mercury
hr	hour
IARC	International Agency for Research on Cancer
IDLH	immediately dangerous to life and health value
in	inch
J	joule, m <sup>2</sup> kg-s, N-m, Pa-m <sup>3</sup> , SI unit of work, energy and heat
K	degree Kelvin, base SI unit of thermodynamic temperature and SI unit of temperature interval
kcal	kilocalorie
kg	kilogram, base SI unit of mass

## 14 - Abbreviations

kJ	kilojoule
kPa	kilopascal
l, L	liter
lbf	pound-force
lel	lower explosion limit
(liq)	liquid phase
long	longitudinal
M	molarity, molar concentration
$\mu\text{m}$	micrometer
m	meter, base SI unit of length
max	maximum
mg	milligram
min	minute
mL	milliliter
mm	millimeter
mN	millinewton
MOhm-m	megohm-meter, $10^6$ ohm-m
mol	mole, base SI unit of amount of substance
mPa	millipascal
MPa	megapascal
N	newton, $\text{kg}\cdot\text{m}/\text{s}^2$ , SI unit of force and 'weight'
NA	not applicable at standard temperature and pressure or not environmentally relevant
NIOSH	National Institute for Occupational Safety and Health
ng	nanogram
nm	nanometer
nPa	nanopascal
(OC)	open cup flash point tester, kind not specified
OSHA	Occupational Safety and Health Administration
oz	ounce
P	poise, $\text{dyn}\cdot\text{s}/\text{cm}^2$ , cgs unit of (dynamic) viscosity
Pa	Pascal, $\text{N}/\text{m}^2$ , $\text{m}^{-1}\text{kg}\cdot\text{s}^{-2}$ , $\text{J}/\text{m}^3$ , SI unit of pressure and stress
(PE)	photoelectron spectroscopy method to measure ionization potential
pH	negative logarithm of hydrogen ion concentration
(PI)	photoionization method to measure ionization potential
$\text{pK}_a$	negative logarithm of acid dissociation constant
$\text{pK}_{BH}$	negative logarithm of ionization constant of a protonated base
$\text{pK}_s$	negative logarithm of autoprotolysis constant
ppb	parts per billion
ppm	parts per million
$\text{pP}_{\text{oct}}$	negative logarithm of the octonal/water partition coefficient
psi	pound per square inch; correctly: pound-force per square inch ( $\text{lbf}/\text{in}^2$ )
PVA	polyvinyl alcohol
PVC	polyvinyl chloride
RCRA	Resource Conservation and Recovery Act
RTECS	the NIOSH Registry of Toxic Effects of Chemical Substances
s	second, base SI unit of time
(S)	optical spectroscopy method to measure ionization potential
SI	International System of units
(sol)	solid or crystalline phase

St	stokes, cm <sup>2</sup> /s, cgs unit of kinematic viscosity
STEL	short term exposure limit
Syn	synonyms
TLV	ACGIH threshold limit value
TWA	time-weighted average exposure limit
uel	upper explosion limit
V	volt, SI unit of electric potential, potential difference and electromotive force
(VUS)	vacuum ultraviolet spectroscopy method to measure ionization potential
vol%	volume percent
W	Watt, m <sup>2</sup> kg/s <sup>3</sup> , J/s, SI unit of power
wt%	weight percent
>>	very much greater than
>	greater than
=	equal to
≈	approximately equal to
<	less than
<<	very much less than
α	alpha
β	beta
δ	delta
γ	gamma

## 16 - Conversion factors

### Conversion factors

#### Area

$$1 \text{ in}^2 = 6.4516 \text{ cm}^2$$

$$1 \text{ m}^2 = 10.76391042 \text{ ft}^2$$

#### Concentration:

$$\text{ppm} = (\text{mg/m}^3) \times 24.45 / \text{relative molecular mass}$$

$$\text{mg/m}^3 = \text{ppm} \times \text{relative molecular mass} / 24.45$$

#### Density:

$$1 \text{ g/cm}^3 = 1000 \text{ kg/m}^3 = 0.0361273 \text{ lb/in}^3 = 62.428 \text{ lb/ft}^3$$

#### Dipole moment:

$$1 \text{ Debye} = 3.33564 \times 10^{-30} \text{ coulomb-meter}$$

$$1 \text{ coulomb} = 1 \text{ second-ampere} = 2.77778 \times 10^{-4} \text{ Amp-hr}$$

#### Energy, Heat or Work:

$$1 \text{ cal} = 4.1868 \text{ J} = 1.163 \times 10^{-6} \text{ kW-hr} = 3.96832 \times 10^{-3} \text{ BTU}$$

$$1 \text{ BTU} = 1055.06 \text{ J} = 2.930 \times 10^{-4} \text{ kW-hr} = 778.169 \text{ ft-lbf}$$

$$1 \text{ J} = 9.47817 \times 10^{-4} \text{ BTU} = 0.238846 \text{ cal} = 1 \times 10^7 \text{ erg} = 6.2414601 \times 10^{18} \text{ eV}$$

#### Force

$$1 \text{ N} = 0.2248089431 \text{ lbf} = 10^5 \text{ dyn}$$

#### Henry's law constant:

$$1 \text{ kPa-m}^3/\text{mol} = 0.009869 \text{ atm-m}^3/\text{mol}$$

$$1 \text{ atm-m}^3/\text{mol} = 101.3274 \text{ kPa-m}^3/\text{mol}$$

#### Length:

$$1 \text{ m} = 3.28084 \text{ ft} = 39.3701 \text{ in}$$

$$1 \text{ in} = 2.54 \text{ cm (exact)}$$

$$1 \text{ Angstrom unit} = 1 \times 10^{-10} \text{ m} = 0.1 \text{ nm}$$

#### Power

$$1 \text{ W} = 0.735621493 \text{ ft-lb/s} = 3.412141633 \text{ BTU/hr}$$

$$1 \text{ W} = 1.341022090 \times 10^{-3} \text{ horsepower (mechanical)}$$

$$1 \text{ W} = 1.340482574 \times 10^{-3} \text{ horsepower (electrical)}$$

#### Pressure:

$$1 \text{ atm} = 760.002 \text{ mm Hg} = 0.1013274 \text{ MPa} = 14.6960 \text{ psi}$$

$$1 \text{ mm Hg} = 1 \text{ torr} = 133.322 \text{ Pa} = 0.133322 \text{ kPa} = 0.019337 \text{ psi}$$

$$1 \text{ MPa} = 9.86923 \text{ atm} = 145.038 \text{ psi}$$

$$1 \text{ dyn/cm}^2 = 0.1 \text{ Pa}$$

#### Surface tension:

$$1 \text{ dyn/cm} = 0.001 \text{ N/m} = 1 \text{ mN/m}$$

#### Susceptibility:

$$1 \text{ SI unit} = 4\pi \text{ cgs units}$$



Temperature:

$$^{\circ}\text{F} = (1.8 \times ^{\circ}\text{C}) + 32$$

$$^{\circ}\text{C} = (^{\circ}\text{F} - 32)/1.8$$

$$\text{K} = ^{\circ}\text{C} + 273.15 = (^{\circ}\text{F} + 459.67)/1.8$$

Thermal conductivity:

$$1 \text{ cal}/(\text{s-cm-K}) = 418.68 \text{ W}/(\text{m-K})$$

$$1 \text{ BTU}/(\text{hr-ft-}^{\circ}\text{F}) = 1.73073 \text{ W}/(\text{m-K})$$

Viscosity:

$$1 \text{ cP} = 0.001 \text{ kg}/(\text{m-s}) = 0.001 \text{ Pa-s} = 1 \text{ mPa-s}$$

$$1 \text{ cSt} = 0.000001 \text{ m}^2/\text{s}$$

Volume:

$$1 \text{ L} = 0.001 \text{ m}^3 = 1000 \text{ cm}^3 = 1.0566881 \text{ liquid quart} = 0.2641721 \text{ gallon (US)}$$

$$1 \text{ m}^3 = 33.531466672 \text{ ft}^3$$

Weight:

$$1 \text{ lb} = 16 \text{ oz} = 453.59237 \text{ g}$$

$$1 \text{ kg} = 2.204622622 \text{ lb (avoirdupois)}$$

## 18 - Table 1

Table 1. The first priority list of U.S. Environmental Protection Agency top 100 hazardous substances, as published in *Superfund Report*, April 29, 1987. The 100 substances are separated into 4 priority groups of 25 substances each. Group 1 has the highest priority. The report orders substances within each group by Chemical Abstracts Service Registry Number (CAS RN).

CAS RN	SUBSTANCE
PRIORITY GROUP 1	
50-32-8	Benzo[a]pyrene
53-70-3	Dibenzo[a,h]anthracene
56-55-3	Benzo[a]anthracene
57-12-5	Cyanide
60-57-1	Dieldrin/aldrin
67-66-3	Chloroform; trichloromethane.
71-43-2	Benzene,
75-01-4	Vinyl chloride
75-09-2	Methylene chloride
76-44-8	Heptachlor/heptachlor epoxide
79-01-6	Trichloroethene
86-30-6	n-Nitrosodiphenylamine
106-46-7	1,4-Dichlorobenzene
117-81-7	Bis(2-ethylhexyl)phthalate
127-18-4	Tetrachloroethene
205-99-2	Benzo[b]fluoranthene
218-01-9	Chrysene
1745-01-6	p-Dioxin
7439-92-1	Lead
7440-02-0	Nickel
7440-38-2	Arsenic
7440-41-7	Beryllium
7440-43-9	Cadmium
7440-47-3	Chromium
11196-82-5	PCB-1260,54,48,42,32,21,1016

## PRIORITY GROUP 2

56-23-5	Carbon tetrachloride
57-74-9	Chlordane
62-75-9	n-Nitrosodimethylamine
72-55-9	4,4'-DDE, DDT, DDD
75-00-3	Chloroethane
75-27-4	Bromodichloromethane
75-35-4	1,1-Dichloroethene
78-59-1	Isophorone
78-87-5	1,2-Dichloropropane
79-00-5	1,1,2-Trichloroethane
79-34-5	1,1,2,2-Tetrachloroethane
87-86-5	Pentachlorophenol
91-94-1	3,3'-Dichlorobenzidine
92-87-5	Benzidine
107-06-2	1,2-Dichloroethane

108-88-3	Toluene
108-95-2	Phenol
111-44-4	<i>Bis</i> (2-chloroethyl)ether
121-14-2	2,4-Dinitrotoluene
319-84-6	BHC- $\alpha$ , $\gamma$ , $\beta$ , $\delta$
542-88-1	<i>Bis</i> (chloromethyl)ether
621-64-7	n-Nitrosodi-n-propylamine
7439-97-6	Mercury
7440-66-6	Zinc
7782-49-2	Selenium

## PRIORITY GROUP 3

71-55-6	1,1,1-Trichloroethane
74-87-3	Chloromethane
75-21-8	Oxirane
75-25-2	Bromoform
75-34-3	1,1-Dichloroethane
84-74-2	Di-n-butyl phthalate
88-06-2	2,4,6-Trichlorophenol
91-20-3	Naphthalene
98-95-3	Nitrobenzene
100-41-4	Ethylbenzene
107-02-8	Acrolein
107-13-1	Acrylonitrile
108-90-7	Chlorobenzene
118-74-1	Hexachlorobenzene
122-66-7	1,2-Diphenylhydrazine
124-48-1	Chlorodibromomethane
156-60-5*	1,2-Trans-dichloroethene
193-39-5	Indeno(1,2,3-cd)pyrene
606-20-2	2,6-Dinitrotoluene
1330-20-7	Total Xylenes
7221-93-4	Endrin aldehyde/endrin
7440-22-4	Silver
7440-50-8	Copper
7664-41-7	Ammonia
8001-35-2	Toxaphene

## PRIORITY GROUP 4

51-28-5	2,4-Dinitrophenol
59-50-7	p-Chloro-m-cresol
62-53-3	Aniline
65-85-0	Benzoic acid
67-72-1	Hexachloroethane
74-83-9	Bromomethane
75-15-0	Carbondisulfide
75-64-9	Fluorotrichloromethane
75-71-8	Dichlorodifluoromethane
78-93-3	2-Butanone

\* Published incorrectly in *Superfund Report* as CAS RN 156-60-6.

20 - Table 1

84-66-2	Diethyl phthalate
85-01-8	Phenanthrene
87-68-3	Hexachlorobutadiene
95-48-7	Phenol, 2-methyl
95-50-1	1,2-Dichlorobenzene
105-67-9	2,4-dimethylphenol
108-10-1	2-pentanone,4-methyl
120-82-1	1,2,4-Trichlorobenzene
120-83-2	2,4-Dichlorophenol
123-91-1	1,4-Dioxane
131-11-3	Dimethyl phthalate
206-44-0	Fluoranthene
534-52-1	4,6-Dinitro-2-methylphenol
541-73-1	1,3-Dichlorobenzene
7440-28-0	Thallium

Table 2. Ranking of top 20 organic ground water contaminants based on number of sites at which each contaminant was detected, adapted from Plumb and Pitchford (1985). Rank of one occurs most often.

<u>Rank</u>	<u>Substance</u>	<u>CAS RN</u>	<u>Molecular formula</u>
1	Trichloroethene	79-01-6	C <sub>2</sub> HCl <sub>3</sub>
2	Dichloromethane	75-09-2	CH <sub>2</sub> Cl <sub>2</sub>
3	Tetrachloroethene	127-18-4	C <sub>2</sub> Cl <sub>4</sub>
4	Toluene	108-88-3	C <sub>7</sub> H <sub>8</sub>
5	1,1-Dichloroethane	75-34-3	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>
6	<i>Bis</i> (2-ethylhexyl)phthalate	117-81-7	C <sub>24</sub> H <sub>38</sub> O
7	Benzene	71-43-2	C <sub>6</sub> H <sub>6</sub>
8	<i>trans</i> -1,2-Dichloroethene	156-60-5	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>
9	1,1,1-Trichloroethane	71-55-6	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>
10	Chloroform	67-66-3	CHCl <sub>3</sub>
11	Ethylbenzene	100-41-4	C <sub>8</sub> H <sub>10</sub>
12	1,2-Dichloroethane	107-06-2	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>
13	1,1-Dichloroethene	75-35-4	C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>
14	Phenol	108-95-2	C <sub>6</sub> H <sub>6</sub> O
15	Vinyl chloride	75-01-4	C <sub>2</sub> H <sub>3</sub> Cl
16	Chlorobenzene	108-90-7	C <sub>6</sub> H <sub>5</sub> Cl
17	Dibutyl phthalate	84-74-2	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>
18	Naphthalene	91-20-3	C <sub>10</sub> H <sub>8</sub>
19	Chloroethane	75-00-3	C <sub>2</sub> H <sub>5</sub> Cl
20	Acetone	67-64-1	C <sub>3</sub> H <sub>6</sub> O

## 22 - Table 3

Table 3. The 108 selected hazardous substances ordered by the Chemical Abstracts Service Registry Number (CAS RN). Common synonyms are noted with the name used in this report listed first. The Chemical Abstracts Service recommendations for a common name are underlined (American Chemical Society 1980, Chemical Abstracts Service Registry Handbook - Common Names: ACS, Columbus, OH; names section, 3386 p. or 38 fiche; numbers section, 6638 p. or 74 fiche). Trademark notations are not included. Note: Some synonyms may be ambiguously or incorrectly applied in the literature and therefore in this report.

<u>CAS RN</u>	<u>Synonyms</u>
50-29-3	DDT * <u>Benzene, 1,1'-(2,2,2-trichloro-ethylidene)bis[4-chloro-</u> * Aavero-extra * Agritan * Anofex * Arkotine * Azotox M-33 * $\alpha,\alpha$ -bis(p-chlorophenyl)- $\beta,\beta,\beta$ -trichloroethane * 1,1'-bis(p-Chlorophenyl)-2,2,2-trichloroethane * 2,2-bis(p-Chlorophenyl)-1,1,1-trichloroethane * Bosan supra * Bovidermol * Chlorophenotene * Chlorophenothan * Chlorophenothane * Chlorphenothan * Chlorphenotoxum * Citox * Clofenotan * Clofenotane * p,p'-DDT * 4,4'-DDT * Dedelo * Deoval * Detox * Detoxan * Dibonan * Dibovin * Dichlorodiphenyltrichloroethane * p,p'-Dichlorodiphenyltrichloroethane * 4,4'-Dichlorodiphenyltrichloroethane * Dicophane * Didigam * Didimac * diphenyltrichloroethane * Dodat * Dykol * ENT-1506 * Estonate * Genitox * Gesafid * Gesapon * Gesarex * Gesarol * Guesapon * Guesarol * Gyron * Havero-extra * Hildit * Ivoran * Ixodex * Kopsol * Micro DDT 75 * Mutoxan * Mutoxin * NA-2761 * NCI-C00464 * Neocid * Neocidol (solid) * OMS-16 * Parachlorocidum * PEB <sub>1</sub> * Pentachlorin * Pentech * Penticidum * Ppzeidan * R50 * RCRA Waste Number U061 * Rukseam * Santobane * Tafidex * Tech DDT * Trichlorobis(4-chlorophenyl)ethane * 1,1,1-Trichloro-2,2-bis(p-chlorophenyl)ethane * 1,1,1-Trichloro-2,2-di(4-chlorophenyl)-ethane * Zeidane * Zerdane *
50-32-8	<u>Benzo[a]pyrene</u> * Benzo(d,e,f)chrysene * 1,2-benzpyrene * 1,2-benzopyrene * 3,4-Benzopyrene * 6,7-Benzopyrene * Benz(a)pyrene * 3,4-Benz(a)pyrene * 3,4-Benzypyrene * BP * 3,4-BP* B(a)P * RCRA Waste Number U022 *
51-28-5	2,4-Dinitrophenol * <u>Phenol, 2,4-dinitro-</u> * Aldifen * Chemox PE * $\alpha$ -Dinitrophenol * DNP * 2,4-DNP * Fenoxyl carbon n * 1-Hydroxy-2,4-dinitrobenzene * Maroxol-50 * Nitro kleenup * Nitrophen * Nitrophen * NSC 1532 * Phenol, $\alpha$ -Dinitro- * RCRA Waste Number P048 * Solfo black B * Solfo black BB * Solfo black 2B supra * Solfo black G * Solfo black SB * Tertrosulphur black PB * Tertrosulphur PBR *
53-70-3	<u>Dibenz[a,h]anthracene</u> * 1,2:5,6-Benzanthracene * DBA * DB(a,h)A * 1,2,5,6-DBA * 1,2:5,6-Dibenzanthracene * 1,2:5,6-Dibenz(a)anthracene * Dibenzo(a,h)anthracene * 1,2:5,6-Dibenzoanthracene * RCRA Waste Number U063 *
56-23-5	Carbon tetrachloride * <u>Methane, tetrachloro-</u> * Asordin * Benzinoform * Carbona * Carbon chloride * Carbon tet * ENT 4705 * ENT 27164 * Fasciolin * Flukoids * Freon 10 * Katarine * Methane tetrachloride * Necatorina * Necatorine * Perchloromethane * Phoenipine * Pyrene * R-10 * RCRA Waste

	Number U211 * Spectral * Tetra * Tetrachlorocarbon * Tetrachloromethane * Tetracol * Tetrafinol * Tetraform * Tetrasol * UN 1846 (DOT) * Univerm * Vermoestricid *
56-55-3	<u>Benz[a]anthracene</u> * B(a)A * BA * Benzanthracene * 1,2-Benz(a)anthracene * 1,2-Benzanthracene * Benzanthrene * 1,2-Benzanthrene * Benzo(a)anthracene * Benzoanthracene * 1,2-Benzoanthracene * Benzo(a)phenanthrene * Benzo(b)phenanthrene * 2,3-Benzophenanthrene * 2,3-Benzphenanthrene * Naphthanthracene * RCRA Waste Number U018 * Tetraphene *
57-74-9	Chlordane * <u>4,7-Methano-1H-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-</u> * Belt * CD-68 * $\gamma$ -Chloridan * gamma-Chlordan * Chlorindan * chlorodane * Corodane * Cortilan-neu * Dowklor * ENT 9932 * ENT 25,552-x * HCS-3260 * M-140 * 4,7-Methanoindan, 1,2,4,5,6,7,8,8-octachloro-3a,4,7,7a-tetrahydro- * NCI-C00099 * Niran * Octachlorodihydrodicyclopentadiene * 1,2,4,5,6,7,8,8-Octachloro-2,3,4a,4,7,7a-hexahydro-4,7-methanoindene * 1,2,4,5,6,7,8,8-Octachloro-2,3,4a,4,7,7a-hexahydro-4,7-methano-1H-indene * 1,2,4,5,6,7,8,8-Octachloro-3a,4,7,7a-hexahydro-4,7-methylene indane * Octachloro-4,7-methanohydroindane * Octachloro-4,7-methanotetrahydroindane * 1,2,4,5,6,7,8,8-Octachloro-4,7-methano-3a,4,7,7a-tetrahydroindane * 1,2,4,5,6,7,8,8-Octachloro-3a,4,7,7a-tetrahydro-4,7-methanoindane * 1,2,4,5,6,7,10,10-Octachloro-4,7,8,9-tetrahydro-4,7-methyleneindane * Octachlor * Octaklor * Oktaterr * Ortho-Klor * Synklor * Tat Chlor 4 * Toxichlor * Velsicol 1068 * 1068 *
58-89-9	$\gamma$ -Hexachlorocyclohexane * <u>Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1<math>\alpha</math>,2<math>\alpha</math>,3<math>\beta</math>,4<math>\alpha</math>,5<math>\alpha</math>,6<math>\beta</math>)-</u> * Cyclohexane, 1,2,3,4,5,6-hexachlori-, $\gamma$ - * 666 * Aalindan * Aficide * Agrisol G-20 * Agrocide (2, 7, 6G, III, or WP) * Agronexit * Ameisenmittel merck * Ameisentod * Aparasin * Aphitiria * Aplidal * Arbitex * BBH * Ben-hex * Bentox 10 * Benzene hexachloride * $\gamma$ -Benzene hexachloride * Benzene hexachloride-gamma isomer * Benzene-cis-hexachloride * Benxol * BHC * $\gamma$ -BHC * Celanex * Chloran * Chloresene * Codechine * DBH * Detmol-extrakt * Detox 25 * Devoran * Dol granule * Drill tox-spezial aglukon * ENT 7796 * Entomoxan * Exagama * Fenofom forte * Forlin * Forst-nexen * Gallogama * Gamacarbattox * Gamacid * Gamma-col * Gamene * Gamiso * gamma-Benzene hexachloride * gamma-BHC * gamma-HCH * Gammahexa * Gammexene * gamma-Hexachlor * gamma-Hexachloran * gamma-Hexachlorane * Gammahexane * Gammalin * Gamaphex * Gammater * Gammex * Gammexane * Gammopaz * Gexane * HCC * HCCH * HCH * $\gamma$ -HCH * Heclotox * Hexa * Hexachloran * $\gamma$ -hexachloran * Hexachlorane * $\gamma$ -Hexachlorane * $\gamma$ -hexachlorobenzene * 1 $\alpha$ ,2 $\alpha$ ,3 $\beta$ ,4 $\alpha$ ,5 $\alpha$ ,6 $\beta$ -Hexachlorocyclohexane * Hexachlorocyclohexane gamma-isomer * 1,2,3,4,5,6-hexachlorocyclohexanegamma-isomer * Hexatox * Hexaverm * Hexicide * Hexyclan * HGI * Hortex * Hungaria L-7 * $\gamma$ -Isomer * Inexit * Isotox * Jacutin * Kokotine * Kwell * Lendine * Lentox * Lidenal * Lindafor * Lindagam * Lindagrain * Lindagranox * Lindane * $\gamma$ -Lindane * Lindapoudre * Lindatox * Lindex * Lindosep * Lintox * Linvur * Lorexane * Mglawik L * Milbol 49 * Mszycol * NA 2761 (DOT) * NCI-C00204 * Neo-

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	scabacidol * Nexen FB * Nexit * Nexit-stark * Nexol-E * Nicochloran * Novigam * Omnitox * Ovardiak * Owadziak * Pedraczak * Pflanzol * Quellada * RCRA Waste Number U129 * Sang-gamma * Silvanol * Spritz-Rapidin * Spruehpflanzol * Streunex * TAP 85 * TBH * Tri-6 * Viton *
59-50-7	6-Chloro- <i>m</i> -cresol * <u>Phenol, 4-chloro-3-methyl-</u> * Aptal * Baktol * Baktolan * Canaseptic * <i>p</i> -Chloro- <i>m</i> -cresol * <i>para</i> - Chloro- <i>meta</i> -cresol * <i>p</i> -Chlor- <i>m</i> -cresol * Chlorocresol * <i>p</i> - Chlorocresol * 4-Chloro- <i>m</i> -cresol * 4-Chloro-1-hydroxy-3- methylbenzene * 6-Chloro-3-hydroxytoluene * 4-Chloro-3- hydroxytoluene * 2-Chloro-hydroxytoluene * 2-Chloro-5- methylphenol * 4-Chloro-3-methylphenol * <i>m</i> -Cresol, 4-chloro- * 3-Methyl-4-chlorophenol * Ottafact * Parmetol * Parol * PCMC * Peritonan * Preventol CMK * Raschit * Raschit K * Rasen-Anicon * RCRA Waste Number U039 *
60-57-1	Dieldrin * <u>2,7:3,6-Dimethanonaphth[2,3-<i>b</i>]oxirene,</u> <u>3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-</u> <u>(1a<math>\alpha</math>,2<math>\beta</math>,2a<math>\alpha</math>,3<math>\beta</math>,6<math>\beta</math>,6a<math>\alpha</math>,7<math>\beta</math>,7a<math>\alpha</math>)-</u> * 1,4:5,8- Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-6,7-epoxy- 1,4,4a,5,6,7,8,8a-octahydro-, <i>endo</i> , <i>exo</i> - * Aldrin epoxide * Alvit * Alvit 55 * Compound 497 * Dieldrex * <i>exo</i> -Dieldrin * Dieldrite * Dieldrix * Dielmoth * Dorytox * ENT 16225 * HEOD * Hexachloroepoxyoctahydro- <i>endo</i> , <i>exo</i> -dimethanonaphthalene * 1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a- octahydro-1,4,5,8-dimethanonaphthalene * 3,4,5,6,9,9- hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-2,7:3,6- dimethanonaphth(2,3- <i>b</i> )oxirene * Illoxol * Insecticide number 497 * Insectlack * Kombi-Albertan * Moth Snub D * NA 2761 (DOT) * NCI-C00124 * Octalox * Panoram D-31 * Quintox * RCRA Waste Number P037 * Red Shield * SD 3417 * Termitox *
62-53-3	Aniline * <u>Benzenamine</u> * Aminobenzene * Aminophen * Aniline oil * Arylamine * Anyvim * Benzene, amino * Benzidam * Blue oil * C.I. 76000 * C.I. oxidation base 1 * Cyanol Krystallin * Kyanol * NCI-C03736 * Phenylamine * RCRA Waste Number U012 * UN 1547 (DOT) *
64-17-5	<u>Ethanol</u> * Absolute Ethanol * Alcohol * Algrain * Anhydrol * Anhydrous alcohol * Denatured alcohol * Denatured ethanol * Dehydrated alcohol * Cologne spirit * Cologne spirits (alcohol) (DOT) * Ethanol 200 proof * Ethanol solution (DOT) * Ethyl alcohol * Ethyl alcohol anhydrous * Ethyl hydrate * Ethyl hydroxide * Fermentation alcohol * Grain alcohol * Jaysol * Jaysol S * Methylcarbinol * Molasses alcohol * NCI- C03134 * Potato alcohol * SD alcohol 23-hydrogen * Spirits of wine * Spirt * Tecsol * UN 1170 (DOT) *
64-19-7	<u>Acetic acid</u> * Ethanoic acid * Ethylic acid * Glacial acetic acid * Methane carboxylic acid * Methylformic acid * UN 2789 (DOT) * UN 2790 (DOT) * Pyroligneous acid * Vinegar acid *
65-85-0	<u>Benzoic acid</u> * Benzenecarboxylic acid * Benzeneformic acid * Benzenemethanoic acid * Benzoate * Carboxybenzene * Carboxyl benzene * Dracylic acid * NA 9094 (DOT) * Phenylcarboxylic acid * Phenylformic acid Retarder BA * Retardex * Salvo liquid * Salvo powder * Tenn-plas *
67-56-1	<u>Methanol</u> * Carbinol * Colonial spirit * Columbian spirits



- \* Methyl alcohol \* Methyl hydrate \* Methyl hydroxide \* Methylol \* Monohydroxymethane \* Pyroxylic spirit \* RCRA Waste Number U154 \* UN 1230 (DOT) \* Wood alcohol \* Wood naphtha \* Wood spirit \*
- 67-64-1 Acetone \* 2-Propanone \* Chevron acetone \* Dimethylformaldehyde \* Dimethylketal \* Dimethyl ketone \* DMK \* Ketone propane \*  $\beta$ -Ketopropane \* Methyl ketone \* Propanone \* Pyroacetic acid \* Pyroacetic ether \* RCRA Waste Number U002 \* UN 1090 (DOT) \*
- 67-66-3 Chloroform \* Methane, trichloro- \* Formyl trichloride \* Freon 20 \* Methane trichloride \* Methenyl trichloride \* Methyl trichloride \* NCI-C02686 \* R 20 \* R 20 (refrigerant) \* RCRA Waste Number U044 \* TCM \* Trichloroform \* Trichloromethane \* UN 1888 (DOT) \*
- 67-68-5 Dimethyl sulfoxide \* Methane, sulfinylbis- \* A 10846 \* Deltan \* Demasorb \* Demavet \* Demeso \* Demsodrox \* Dermasorb \* Dimethyl sulphoxide \* Dimexide \* Dipirartril-tropico \* DMS-70 \* DMS-90 \* DMSO \* Dolicur \* Doligur \* Domoso \* Domosol \* Dromisol \* Durasorb \* Gamasol 90 \* Hyadur \* Infiltrina \* M-176 \* Methylsulfinylmethane \* Methyl sulfoxide \* Methylthiomethane \* NSC-763 \* Rimso-50 \* Somipront \* SQ 9453 \* Sulfinylbis[methane] \* Syntexan \* Topsy (rescinded) \*
- 67-72-1 Hexachloroethane \* Ethane, hexachloro- \* Avlothane \* Carbon hexachloride \* Distokal \* Distopan \* Distopin \* Egitol \* Ethane hexachloride \* Ethylene hexachloride \* Falkitol \* Fasciolin \* HCE \* 1,1,1,2,2,2-Hexachloroethane \* Hexachloroethylene \* Mottenhexe \* NA 9037 (DOT) \* NCI-C04604 \* Perchlorethane \* Perchloroethane \* Phenohep \* RCRA Waste Number U131 \*
- 71-43-2 Benzene \* (6)Annulene \* Benzol \* Benzole \* Benzolene \* Bicarburet of hydrogen \* Carbon oil \* Coal naphtha \* Cyclohexatriene \* Mineral naphtha \* Motor benzol \* NCI-C55276 \* Nitration benzene \* Phene \* Phenyl hydride \* Polystream \* Pyrobenzol \* Pyrobenzole \* RCRA Waste Number U019 \* UN 1114 (DOT) \*
- 71-55-6 1,1,1-Trichloroethane \* Ethane, 1,1,1-trichloro- \* Aerothane \* Aerothene \* Aerothene TT \* Baltana \* Chloroetene \* Chloroethene \* Chlorotene \* Chlorothane NU \* Chlorothene \* Chlorothene NU \* Chlorothene VG \* Chlorten \* Genklene \* Inhibisol \* Methylchloroform \* Methyl chloroform \* Methyltrichloromethane \* NCI-C04626 \* RCRA Waste Number U226 \* Solvent III \* Strobane \*  $\alpha$ -T \* 1,1,1-TCA \* 1,1,1-TCE \* Trichloroethane \*  $\alpha$ -Trichloroethane \* Tri-ethane \* UN 2831 (DOT) \*
- 72-20-8 Endrin \* 2,7:3,6-Dimethanonaphth[2,3-b]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-(1a $\alpha$ ,2 $\beta$ ,2a $\beta$ ,3 $\alpha$ ,6 $\alpha$ ,6a $\beta$ ,7 $\beta$ ,7a $\alpha$ )- \* Compound 269 \* 1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-,endo,endo- \* EN 57 \* Endrex \* Endricol \* ENT 17251 \* Experimental insecticide 269 \* Hexachloroepoxyoctahydro-endo-endo-dimethanonaphthalene \* 1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-1,4-endo-endo-5,8-dimethanonaphthalene \* Hexadrin \* Isodrin epoxide \* Mendrin \* NA 2761 \* NCI-C00157 \* Nendrin \*

- Oktanex \* RCRA Waste Number P051 \* SD 3419 \*
- 74-83-9 Bromomethane \* Methane, bromo- \* Bercema \* Brom-o-gas \* Brom-o-gaz \* Curafume \* Dawson 100 \* Detia gas EX-M \* Dowfume \* Dowfume MC-2 \* Dowfume MC-33 \* EDCO \* Embafume \* Fumigant-1 (obs.) \* Halon 1001 \* Haltox \* Iscobrome \* Kayafume \* MB \* M-B-C fumigant \* MBX \* MEBR \* Metafume \* Methogas \* Methyl bromide \* Monobromomethane \* Pestmaster (obs) \* Profume (obs.) \* R40B1 \* RCRA Waste Number U029 \* Rotox \* Terabol \* Terr-o-gas 67 \* Terr-o-gas 100 \* UN 1062 (DOT) \* Zytox \*
- 74-87-3 Chloromethane \* Methane, chloro- \* Artic \* Methyl chloride \* Monochloromethane \* R 40 \* RCRA Waste Number U045 \* UN 1063 (DOT) \*
- 74-90-8 Hydrogen cyanide \* Hydrocyanic acid \* Carbon hydride nitride \* Evercyn \* Formic anammonide \* Formonitrile \* Prussic acid \*
- 75-00-3 Chloroethane \* Ethane, chloro- \* Aethylis \* Aethylis chloridum \* Anodynnon \* Chelen \* Chlorene \* Chlorethyl \* Chloridum \* Chloryl \* Chloryl anesthetic \* Cloretilo \* Ether chloratus \* Ether hydrochloric \* Ether muriatic \* Ethyl chloride \* Hydrochloric ether \* Kelene \* Monochloroethane \* Monochloroethane \* Muriatic ether \* Narcotile \* NCI-C06224 \* UN 1037 (DOT) \*
- 75-01-4 Vinyl chloride \* Ethene, chloro- \* Chloroethene \* 1-Chloroethene \* Chlorethylene \* Chloroethylene \* 1-Chloroethylene \* Ethylene, chloro- \* Ethylene monochloride \* Monochloroethene \* Monochloroethylene \* MVC \* RCRA Waste Number U043 \* Trovidur \* UN 1086 (DOT) \* VCL \* VCM \* Vinyl chloride monomer \* Vinyl C monomer \*
- 75-09-2 Dichloromethane \* Methane, dichloro- \* Aerothene MM \* DCM \* Freon 30 \* Methane dichloride \* Methylene bichloride \* Methylene chloride (DOT) \* Methylene dichloride \* Narkotil \* NCI-C50102 \* R 30 \* RCRA Waste Number U080 \* Solaesthin \* Solmethine \* UN 1593 (DOT) \*
- 75-15-0 Carbon disulfide \* Carbon bisulfide \* Carbon bisulphide \* Carbon disulphide \* Carbon sulfide \* Dithiocarbonic anhydride \* NCI-C04591 \* RCRA Waste Number P022 \* Sulphocarbonic anhydride \* UN 1131 (DOT) \* Weeviltox \*
- 75-21-8 Ethylene oxide \* Oxirane \* Anprolene \* Dihydrooxirene \* Dimethylene oxide \* EO \* Epoxyethane \* 1,2-Epoxyethane \* Ethene oxide \* ETO \* NCI-C50088 \* Oxacyclopropane \* Oxane \* Oxidoethane \*  $\alpha,\beta$ -Oxidoethane \* Oxyfume \* Oxyfume 12 \* T-gas \*
- 75-25-2 Bromoform \* Methane, tribromo- \* Methenyl tribromide \* Methyl tribromide \* NCI-C55130 \* RCRA Waste Number U225 \* Tribromomethane \* UN 2515 (DOT) \*
- 75-34-3 1,1-Dichloroethane \* Ethane, 1,1-dichloro- \* Asymmetrical dichloroethane \* Chlorinated hydrochloric ether \* Dichlorethane \* Dichloroethane \* Ethylidene chloride \* Ethylidene dichloride \* 1,1-ethylidene dichloride \* NCI-C04535 \* RCRA Waste Number U076 \* UN 2362 (DOT) \*
- 75-35-4 1,1-Dichloroethene \* Ethene, 1,1-dichloro- \* asym-dichloroethylene \* 1,1-DCE \* 1,1-dichloroethylene \* Ethylene, 1,1-dichloro- \* NCI-C54262 \* RCRA Waste Number U078 \* UN 1303 (DOT) \* unsym-Dichloroethylene \* VC \* VDC \* Vinylidene

	chloride * Vinylidene chloride II * Vinylidene chloride, inhibited * Vinylidene dichloride * Vinylidine dichloride *
75-69-4	Trichlorofluoromethane * <u>Methane, trichlorofluoro-</u> * Algofrene type 1 * Arcton 9 * Electro-CF 11 * Eskimon 11 * F-11 * F 11B * FC 11 (halocarbon) * FKW 11 * Fluorocarbon no. 11 * Fluorochloroform * Fluorotrichloromethane * Freon 11 * Freon 11A * Freon 11B * Freon HE * Freon MF * Frigen 11 * Frigen 11A * Genetron 11 * Halocarbon 11 * Isceon 11 * Isceon 131 * Isotron 11 * Kaltron 11 * Ledon 11 * Methane, fluorotrichloro- * Monofluorotrichloromethane * NCI-C04637 * Propellant 11 * R 11 (refrigerant) * R 11 (halocarbon) * RCRA Waste Number U121 * Refrigerant 11 * Trichloromonofluormethane * Ucon 11 * Ucon fluorocarbon 11 * Ucon refrigerant 11 *
75-71-8	Dichlorodifluoromethane * <u>Methane, dichlorodifluoro-</u> * Algofrene type 2 * Arcton 6 * Arcton 12 * Difluorodichloromethane * Electro-CF 12 * Eskimon 12 * F-12 * FC 12 * Fluorocarbon-12 * Freon 12 * Frigen 12 * Genetron 12 * Halon * Halon 122 * Isceon 122 * Isotron 12 * Kaiser Chemicals 12 * Ledon 12 * Propellant 12 * R 12 * R 12 (refrigerant) * RCRA Waste Number U075 * Refrigerant 12 * Ucon 12 * Ucon 12/halocarbon 12 * UN 1028 (DOT) *
76-44-8	Heptachlor * <u>4,7-Methano-1H-indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-</u> * Aahepta * Agroceres * Basaklor * 3-Chlorochlordene * Drinox H-34 * E 3314 * ENT 15152 * GPKh * H34 * Hepta * Heptachlorane * 3,4,5,6,7,8,8-Heptachlorodicyclopentadiene * 3,4,5,6,7,8,8a-Heptachlorodicyclopentadiene * 1,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-endo-methanoindene * 1,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindane * 1,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindene * Heptachlorodicyclopentadiene * Heptagran * Heptagranox * Heptamak * Heptamul * Heptasol * Heptox * 4,7-Methanoindene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro- * NA 2761 * NCI-C00180 * RCRA Waste Number P059 * Rhodiachlor * Soleptax * Velsicol 104 * Velsicol heptachlor *
78-59-1	Isophorone * <u>2-Cyclohexen-1-one, 3,5,5-trimethyl-</u> * Isoacetophorone * Isoforon * Isooctaphenone * Isophoron * $\alpha$ -Isophoron * $\alpha$ -Isophorone * NCI-C55618 * 1,1,3-trimethyl-3-cyclohexene-5-one * 3,5,5-Trimethyl-5-cyclohexen-1-one * 3,5,5-Trimethyl-2-cyclohexene-1-one * Trimethylcyclohexenone * UN 1224 (DOT) *
78-87-5	1,2-Dichloropropane * <u>Propane, 1,2-dichloro-</u> * $\alpha,\beta$ -Dichloropropane * ENT 15406 * NCI-C55141 * Propylene chloride * Propylene dichloride * $\alpha,\beta$ -Propylene dichloride * RCRA Waste Number U083 *
78-93-3	<u>2-Butanone</u> * Butanone * 3-Butanone * Ethyl methyl ketone * Meetco * MEK * Methyl acetone * Methyl ethyl ketone * RCRA Waste Number U159 * UN 1193 (DOT) * UN 1232 (DOT) *
79-00-5	1,1,2-Trichloroethane * <u>Ethane, 1,1,2-trichloro-</u> * Ethane trichloride * NCI-C04579 * RCRA Waste Number U227 * RCRA Waste Number U359 * $\beta$ -T * beta-T * 1,1,2-TCA * 1,1,2-Trichlorethane * $\beta$ -Trichloroethane * beta-Trichloroethane * 1,2,2-Trichloroethane * Vinyl trichloride *

- 79-01-6 Trichloroethene \* Ethene, trichloro- \* Acetylene trichloride \* Algylen \* Anamenth \* Benzinol \* Blacosolv \* Blancosolv \* Cecolene \* Chorilen \* 1-Chloro-2,2-dichloroethylene \* Chlorylea \* Chlorylen \* Chorylen \* Circosolv \* Crawhaspol \* Densinfluat \* 1,1-Dichloro-2-chloroethylene \* Dow-Tri \* Dukeron \* Ethinyl trichloride \* Ethylene trichloride \* Ethylene, trichloro- \* Flek-flip \* Flock-flip \* Fluata \* Gemalgene \* Germalene \* Germalgene \* Lanadin \* Lethurin \* Narcogen \* Narkogen \* Narkosoid \* NCI-C04546 \* Nialk \* Perm-a-chlor \* Perm-a-clor \* Petzinol \* Philex \* RCRA Waste Number U228 \* TCE \* Threthylen \* Threthylene \* Trethylene \* Tri \* Triad \* Trial \* Triasol \* Trichloran \* Trichloren \* Trichloroethylene \* 1,1,2-Trichloroethylene \* 1,2,2-Trichloroethylene \* 1,1,2-Trichloroethene \* 1,2,2-Trichloroethene \* Tri-clene \* Tricloren \* Trielene \* Trielin \* Triklone \* Trilen \* Trilene \* Triline \* Trimar \* Triol \* Tri-plus \* Tri-plus M \* UN 1710 (DOT) \* Vestrol \* Vextrol \* Vitran \* Westrosol \*
- 79-34-5 1,1,2,2-Tetrachloroethane \* Ethane, 1,1,2,2-tetrachloro- \* Acetylene tetrachloride \* Bonoform \* Cellon \* 1,1-Dichloro-2,2-dichloroethane \* Ethane tetrachloride \* NCI-C03554 \* RCRA Waste Number U209 \* TCE \* Tetrachlorethane \* Tetrachloroethane \* sym-Tetrachloroethane \* UN 1702 (DOT) \* Westron \*
- 84-66-2 Diethyl phthalate \* 1,2-Benzenedicarboxylic acid, diethyl ester \* Anozol \* Diethylphthalate \* Diethyl-o-phthalate \* DEP \* Estol 1550 \* Ethyl phthalate \* NCI-C60048 \* Neantine \* Palatinol A \* Phthalic acid, diethyl ester \* Phthalol \* Placidol E \* RCRA Waste Number U088 \* Solvanol \* Unimoll DA \*
- 84-74-2 Dibutyl phthalate \* 1,2-Benzene-dicarboxylic acid, dibutyl ester \* o-Benzenedicarboxylic acid dibutyl ester \* Benzene-o-dicarboxylic acid di-n-butyl ester \* Butyl phthalate \* n-Butyl phthalate \* Celluflex DBP \* DBP \* Dibutyl 1,2-benzenedicarboxylate \* Dibutyl ester phthalic acid \* Di-n-butyl phthalate \* Elaol \* Ergoplast FDB \* Genoplast B \* Hexaplas M/B \* NA 9095 \* Palatinol C \* Phthalic acid, dibutyl ester \* Polycizer DBP \* PX 104 \* RCRA Waste Number U069 \* RC plasticizer DBP \* Staflex DBP \* Unimoll DB \* Witicizer 300 \*
- 85-01-8 Phenanthrene \* Phenanthren \* Phenantrin \*
- 86-30-6 n-Nitrosodiphenylamine \* Benzenamine, N-nitroso-N-phenyl- \* Curetard A \* Delac J \* Diphenylamine, N-nitroso- \* Diphenylnitrosamine \* Diphenyl N-nitrosoamine \* N,N-Diphenylnitrosamine \* Naugard TJB \* NCI-C02880 \* NDPA \* NDPHA \* Nitrosodiphenylamine \* N-Nitroso-N-phenylaniline \* Nitrous diphenylamide \* Redax \* Retarder J \* TJB \* Vulcalent A \* Vulcatard \* Vulcatard A \* Vulkalent A \* Vultrol \*
- 87-68-3 Hexachlorobutadiene \* 1,3-Butadiene, 1,1,2,3,4,4-hexachloro- \* C 46 \* Dolen-pur \* GP-40-66:120 \* HCB \* HCBD \* 1,3-Hexachlorobutadiene \* Hexachloro-1,3-butadiene \* Hexachlorobuta-1,3-diene \* 1,1,2,3,4,4-Hexachloro-1,3-butadiene \* Perchlorobutadiene \* RCRA Waste Number U128 \* UN 2279 (DOT) \*
- 87-86-5 Pentachlorophenol \* Phenol, pentachloro- \* Acutox \* Chem-penta \* Chem-tol \* Chlon \* Chlorophen \* Cryptogil OL \*

	Dowside EC-7 * Dowside G Dowside 7 * Dowicide 7 * Dow pentachlorophenol DP-2 antimicrobial * Durotox * EP 30 * Fungifen * Glazd Penta * Grundier arbezol * Lauxtol * Lauxtol A * Lioprem * Monsanto Penta * Moosuran * NA 2020 (DOT) * NCI-C54933 * NCI-C55378 * NCI-C56655 * PCP * PCP (pesticide) * Penchlorol * Penta * Pentachlorofenol * Pentachlorophenate * 2,3,4,5,6-Pentachlorophenol * Pentachlorophenol, Dowicide EC-7 * Penta-chlorofendo * Pentachlorophenol, DP-2 * Pentacon * Penta-kil * Pentasol * Penwar * Peratox * Permacide * Permagard * Permasan * Permattox DP-2 * Permattox Penta * Permite * PKhF * Prevenol P * Prilttox * RCRA Waste Number U242 * Santobrite * Santophen * Santophen 20 * Sinituho * Term-i-trol *Thompson's Wood Fix * Weedone * Witophen * Witophen P *
88-06-2	2,4,6-Trichlorophenol * <u>Phenol, 2,4,6-trichloro-</u> * Dowside 2S * Dowside 25 * Dowicide 2S * NCI-C02904 * Omal * Phenachlor * RCRA Waste Number U231 * RCRA Waste Number F027 * 2,4,6-TCP * 2,4,6-TCP-Dowicide 25 UN 2020 (dot) *
91-20-3	<u>Naphthalene</u> * Albocarbon * Camphor tar * Dezodorator * Mighty 150 * Mighty RD1 * Moth balls * Moth flakes * Naphthalin * Naphthaline * Naphthene * Naphthalene, molten * NCI-C52904 * RCRA Waste Number U165 * Tar camphor * UN 1334 (DOT) * UN 2304 (DOT) * White tar *
91-22-5	Quinoline * 1-Azanaphthalene * B-500 * 1-Benzanine * 1- Benzazine * 1-Benzine * Benzo(b)pyridine * Benzopyridine * Chinoleine * Chinoline * Leucol * Leucoline * Leukol * Quinolin * UN 2656 (DOT) * USAF EK-218 *
92-87-5	Benzidine * <u>[1,1'-Biphenyl]-4,4'-diamine</u> * Benzidine base * <i>p,p'</i> -Bianiline * <i>P,P'</i> -Bianiline * 4,4'-Bianiline * Biphenyl, 4,4'-diamino- * 4,4'-Biphenyldiamine * 4,4'- Biphenylenediamine * C.I. 37225 * C.I. azoic diazo component 112 * 4,4'-Diaminobiphenyl * <i>p,p'</i> -Diaminobiphenyl * 4,4'- Diamino-1,1'-biphenyl * <i>p</i> -Diaminodiphenyl * <i>para</i> - Diaminodiphenyl * 4,4'-Diaminodiphenyl * <i>p,p'</i> -Dianiline * 4,4'-Diphenylenediamine * Fast Corinth Base B * NCI-C03361 * RCRA Waste Number U021 * UN 1885 (DOT) *
95-47-6	<i>o</i> -Xylene * <u>Benzene, 1,2-dimethyl-</u> * 1,2-Dimethylbenzene * <i>o</i> -Dimethylbenzene * <i>o</i> -Methyltoluene * UN 1307 (DOT) * 1,2- Xylene * 2-Xylene * <i>ortho</i> -Xylene * <i>o</i> -Xylol *
95-48-7	<i>o</i> -Cresol * <u>Phenol, 2-methyl-</u> * 2-cresol * <i>o</i> -Cresylic acid * 1-Hydroxy-2-methylbenzene * 2-Hydroxytoluene * <i>o</i> - Hydroxytoluene * <i>o</i> -Kresol * 2-Methylbenzenol * 2-Methylphenol * <i>o</i> -Methylphenol * <i>o</i> -Methylphenylol * <i>ortho</i> -Cresol * <i>o</i> - Oxytoluene * RCRA Waste Number U052 * <i>o</i> -Toluol * UN 2076 (DOT) *
95-50-1	1,2-Dichlorobenzene * <u>Benzene, 1,2-dichloro-</u> * Chloroben * Chloroden * DCB * <i>o</i> -DCB * 1,2-DCB * <i>o</i> -Dichlorbenzene * <i>o</i> - Dichlor benzol * <i>ortho</i> -Dichlorobenzene * Dichlorobenzene * <i>o</i> -Dichlorobenzene * Dichlorobenzene, <i>ortho</i> , liquid * <i>o</i> - Dichlorobenzol * Dilantin DB * Dilatin DB * Dizene * Dowtherm E * NCI-C54944 * ODB * ODCB * Orthodichlorobenzene * Orthodichlorobenzol * RCRA Waste Number U070 * Special termite fluid * Termitkil * UN 1591 (DOT) *
98-95-3	Nitrobenzene * <u>Benzene, nitro-</u> * Essence of mirbane *

	Essence of myrbane * Mirbane oil * NCI-C60082 *
	Nitrobenzene, liquid * Nitrobenzol * Nitrobenzol, liquid *
	Oil of bitter almonds * Oil of mirbane * Oil of myrbane *
	RCRA Waste Number U169 * UN 1662 (DOT) *
100-41-4	Ethylbenzene * <u>Benzene, ethyl</u> * EB * Ethyl benzene *
	Ethylbenzol * NCI-C56393 * Phenylethane * UN 1174 (DOT)
105-67-9	2,4-Xylenol * <u>Phenol, 2,4-dimethyl-</u> * 2,4-Dimethylphenol *
	4,6-Dimethylphenol * 2,4-DMP * 1-Hydroxy-2,4-dimethylbenzene
	* 4-Hydroxy-1,3-dimethylbenzene * RCRA Waste Number U101 * UN
	2261 (DOT) * 1,3,4 Xylenol * <i>m</i> -Xylenol * ( <i>as</i> )( <i>m</i> )-Xylenol *
106-42-3	<i>p</i> -Xylene * <u>Benzene, 1,4-dimethyl-</u> * Chromar * 1,4-
	Dimethylbenzene * <i>p</i> -Dimethylbenzene * <i>p</i> -Methyltoluene *
	Scintillar * UN 1307 (DOT) * 1,4-Xylene * 4-Xylene * <i>para</i> -
	Xylene * <i>p</i> -Xylol *
106-46-7	1,4-Dichlorobenzene * <u>Benzene, 1,4-dichloro-</u> * <i>p</i> -
	Chlorophenyl chloride * Di-chloricide * 1,4-DCB * <i>p</i> -
	Dichlorobenzene * Dichlorobenzene, para, solid * <i>p</i> -
	Dichlorobenzol * Dichlorocide * Evola * Globol * NCI-C54955 *
	Paracide * Para Crystals * Paradi * Paradichlorobenzene *
	Paradichlorobenzol * Paradow * Paramoth * Paranuggets *
	Parazene * Parodi * PDB * PDCB * Persia-perazol * RCRA Waste
	Number U070 * RCRA Waste Number U071 * RCRA Waste Number U072
	* Santochlor * UN 1592 (DOT)
106-93-4	1,2-Dibromoethane * <u>Ethane, 1,2-dibromo-</u> * Aadibroom *
	Bromofume * Bromofume 40 * Celmide * DBE * Dibromoethane *
	<i>sym</i> -Dibromoethane * $\alpha,\beta$ -Dibromoethane * Dowfume EDB * Dowfume
	W-8 * Dowfume W-85 * Dowfume W-90 * Dowfume W-100 * EDB *
	EDB-85 * E-D-Bee * ENT 15349 * Ethylene bromide * Ethylene
	dibromide * 1,2-Ethylene dibromide * Fumo-gas * Glycol
	bromide * Glycol dibromide * Iscobrome D * Kopfume * NCI-
	C00522 * Nefis * Nephis * Pestmaster * Pestmaster EDB-85 *
	RCRA Waste Number U067 * Sanhyuum * Soilbrom-40 * Soilbrom-85
	* Soilbrom-90 * Soilbrom-100 * Soilbrome-85 * Soilbrom-90EC *
	Soilfume * UN 1605 (DOT) * Unifume *
107-02-8	Acrolein * <u>2-Propenal</u> * Acquinite * Acraldehyde * <i>trans</i> -
	Acrolein * Acrolein, inhibited * Acrylaldehyde * Acrylic
	aldehyde * Allyl aldehyde * Aqualin * Aqualine * Biocide *
	Crolean * Ethylene aldehyde * Magnacide * Magnacide H * NSC
	8819 * Propenal * Prop-2-en-1-al * 2-Propen-1-one * Propylene
	aldehyde * RCRA Waste Number P003 * Slimicide * UN 1092 (DOT)
	*
107-06-2	1,2-Dichloroethane * <u>Ethane, 1,2-dichloro-</u> * 1,2-
	Bichloridiethane * 1,2-bichloroethane * Borer sol * Brocide *
	1,2-DCE * Destruoxol Borer-sol * Dichloremulsion * 1,2-
	Dichloroethane * Di-chlor-mulsion * $\alpha,\beta$ -Dichloroethane * <i>sym</i> -
	Dichloroethane * Dichloroethylene * Dutch liquid * Dutch oil
	* EDC * ENT 1656 * Ethane dichloride * Ethene dichloride *
	Ethylene chloride * Ethylene dichloride * 1,2-Ethylene
	dichloride * Freon 50 * Glycol dichloride * NCI-C00511 * RCRA
	Waste Number U077 * UN 1184 (DOT) *
107-13-1	Acrylonitrile * <u>2-Propenenitrile</u> * Acritet * Acrylon *
	Acrylonitrile, inhibited * Acrylonitrile monomer * AN *
	Carbacryl * Cyanoethylene * ENT 54 * Fumigrain * Fumigrain *
	Miller's Fumigrain * Nitrile propenoic acid * Propenenitrile

- \* RCRA Waste Number U009 \* TL 314 \* UN 1093 (DOT) \* VCN \*  
Ventox \* Vinyl cyanide \*
- 107-21-1 Ethylene glycol \* 1,2 Ethanediol \* 1,2 Dihydroxyethane \*  
Ethylene alcohol \* Ethylene dihydrate \* Fridex \* Glycol \*  
Glycol alcohol \* 2-Hydroxyethanol \* Macrogol 400 BPC \*  
Monoethylene glycol \* NCI-C00920 \* Ramp \* Tescol \* Ucar 17 \*
- 108-10-1 4-Methyl-2-pentanone \* 2-Pentanone, 4-methyl- \* Hexanone \*  
Hexone \* Isobutyl methyl ketone \* Isopropylacetone \* Methyl  
isobutyl ketone \* 2-Methyl-4-pentanone \* 2-Methylpropyl  
methyl ketone \* MIBK \* MIK \* RCRA Waste Number U161 \* Shell  
MIBK \* UN 1245 (DOT) \*
- 108-38-3 *m*-Xylene \* Benzene, 1,3-dimethyl- \* 1,3-Dimethylbenzene \*  
*m*-Dimethylbenzene \* *m*-Methyltoluene \* UN 1307 (DOT) \* 1,3-  
Xylene \* 3-Xylene \* *meta*-Xylene \* *m*-Xylol \* Xylol \*
- 108-88-3 Toluene \* Benzene, methyl- \* Antisal 1A \* Methacide \*  
Methane, phenyl- \* Methylbenzene \* Methylbenzol \* NCI-C07272  
\* Phenylmethane \* RCRA Waste Number U220 \* Toluol \* Tolu-sol  
\* UN 1294 (DOT) \*
- 108-90-7 Chlorobenzene \* Benzene, chloro- \* Benzene chloride \*  
Chlorbenzene \* Chlorbenzol \* Chlorobenzol \* MCB \*  
Monochlorbenzene \* Monochlorbenzol \* Monochlorobenzene \* NCI-  
C54886 \* Phenyl chloride \* RCRA Waste Number U037 \* Tetrosin  
SP \* UN 1134 (DOT) \*
- 108-95-2 Phenol \* Baker's P and S liquid and ointment \* Benzenol \*  
Carbolic acid \* Hydroxybenzene \* Monohydroxybenzene \*  
Monophenol \* NA 2821 (DOT) \* NCI-C50124 \* Oxybenzene \* Phenic  
acid \* Phenol alcohol \* Phenol, molten \* Phenol, liquid or  
solution \* Phenyl hydrate \* Phenyl hydroxide \* Phenylic acid  
\* Phenylic alcohol \* RCRA Waste Number U188 \* UN 1671 (solid)  
(DOT) \* UN 2312 (molten) (DOT) \* UN 2821 (solution) (DOT) \*
- 110-82-7 Cyclohexane \* Benzene hexahydride \* Hexahydrobenzene \*  
Hexamethylene \* Hexanaphthene \*
- 111-44-4 *Bis*(2-chloroethyl) ether \* Ethane, 1,1'-oxybis[2-chloro- \*  
BCEE \* *bis*( $\beta$ -chloroethyl) ether \* *bis*(chloro-2-ethyl) oxide \*  
Chlorex \* 1-Chloro-2-( $\beta$ -chloroethyloxy)ethane \* Chloroethyl  
ether \* 2-Chloroethyl ether \* DCEE \* Dichloroether \* 2,2'-  
Dichlorethyl ether \*  $\beta,\beta$ -Dichlorodiethyl ether \* 2,2'-  
Dichlorodiethyl ether \* Dichloroethyl ether \*  $\beta,\beta'$ -  
Dichloroethyl ether \* 2,2'-Dichloroethyl ether \* *sym*-  
Dichloroethyl ether \* Di( $\beta$ -chloroethyl) ether \* Di(2-  
chloroethyl) ether \* Dichloroethyl oxide \* ENT 4504 \* 1,1'-  
Oxybis(2-chloro)ethane \* 1,1'-Oxibis[2-chloroethane] \* RCRA  
Waste Number U025 \* UN 1916 (DOT) \*
- 117-81-7 *Bis*(2-ethylhexyl) phthalate \* 1,2-Benzenedicarboxylic  
acid, bis(2-ethylhexyl) ester \* BEHP \* *bis*(2-ethylhexyl)-1,2-  
benzenedicarboxylate \* *Bis*(2-ethylhexyl) ester phthalic acid  
\* Bisoflex 81 \* Bisoflex DOP \* Compound 889 \* DAF 68 \* DEHP \*  
Di(ethylhexyl) phthalate \* Di(2-ethylhexyl) phthalate \* Di(2-  
ethylhexyl) *ortho*-phthalate \* Dioctyl phthalate \* Di-sec-  
octyl phthalate \* DOP \* Ergoplast FDO \* Ethylhexyl phthalate  
\* 2-Ethylhexyl phthalate \* Eviplast 80 \* Eviplast 81 \*  
Fleximel \* Flexol DOP \* Flexol plasticizer DOP \* Good-rite GP  
264 \* Hatcol DOP \* Hercoflex 260 \* Kodaflex DOP \* Mollan O \*  
NCI-C52733 \* Nuoplaz DOP \* Octoil \* Octyl phthalate \*

	Palatinol AH * Phthalic acid, bis(2-ethylhexyl) ester *
	Phthalic acid dioctyl ester * Pittsburgh PX-138 * Platinol AH
	* Platinol DOP * RC plasticizer DOP * RCRA Waste Number U028
	* Reomol DOP * Reomol D 79P * Sicol 150 * Staflex DOP *
	Truflex DOP * Vestinol AH * Vinicizer 80 * Witcizer 312 *
118-74-1	Hexachlorobenzene * <u>Benzene, hexachloro-</u> * Amatin *
	Anticarie * Bunt-cure * Bunt-no-more * Co-op hexa * Granox NM
	* HCB * Hexa C.B. * Hexachlorbenzene * Julin's carbon
	chloride * No Bunt * No Bunt 40 * No Bunt 80 * No Bunt liquid
	* Pentachlorophenyl chloride * Perchlorobenzene * Phenyl
	perchloryl * Sanocide * Smut-go * RCRA Waste Number U127 *
	Sanocid * Snieciotox * UN 2729 (DOT) *
120-82-1	1,2,4-Trichlorobenzene * <u>Benzene, 1,2,4-trichloro-</u> *
	Hostetex L-PEC * 1,2,4-TCB * unsym-Trichlorobenzene * 1,2,5-
	Trichlorobenzene * 1,3,4-Trichlorobenzene * 1,2,4-
	Trichlorobenzol * UN 2321 (DOT) *
120-83-2	2,4-Dichlorophenol * <u>Phenol, 2,4-dichloro-</u> * 3-Chloro-4-
	hydroxychlorobenzene * DCP * 2,4-DCP * 2,4-
	Dichlorohydroxybenzene * 4,6-Dichlorohydroxybenzene * 4,6-
	Dichlorophenol * NCI-C55345 * RCRA Waste Number U081 *
121-14-2	2,4-Dinitrotoluene * <u>Benzene, 1-methyl-2,4-dinitro-</u> * 2,4-
	Dinitrotoluol * DNT * 2,4-DNT * 1-Methyl-2,4-dinitrobenzene *
	NCI-C01865 * RCRA Waste Number U105 * Toluene, 2,4-dinitro- *
123-91-1	<u>1,4-Dioxane</u> * Diethylene dioxide * 1,4-Diethylene dioxide
	* Diethylene ether * Diethylene oxide * Di(ethylene oxide) *
	Diokan * 1,4-Dioxacyclohexane * Dioxan * Dioxane * Dioxane-
	1,4 * p-Dioxane * p-Dioxin, tetrahydro- * Dioxyethylene ether
	* Glycol ethylene ether * NCI-C03689 * RCRA Waste Number U108
	* Tetrahydro-p-dioxin * Tetrahydro-1,4-dioxin * UN 1165 (DOT)
	*
124-48-1	Dibromochloromethane * <u>Methane, dibromochloro-</u> * CDBM *
	Chlorodibromomethane * Dibromomonochloromethane *
	Monochlorodibromomethane * NCI-C55254 *
127-18-4	Tetrachloroethene * <u>Ethene, tetrachloro-</u> * Ankilostin *
	Antisol 1 * Carbon bichloride * Carbon dichloride * Dee-Solv
	* Didakene * Dow-per * ENT 1860 * Ethylene tetrachloride *
	Fedal-UN * NCI-C04580 * Nema * PCF * PER * Perawin * PERC *
	Perchlor * Perchlorethylene * Perchloroethylene * Perclene *
	Perclene D * Percosolve * Perk * Perklone * Persec * RCRA
	Waste Number U210 * Tetlen * Tetracap * Tetrachlorethylene *
	Tetrachloroethylene * 1,1,2,2-Tetrachloroethylene * Tetraleno
	* Tetralex * Tetravec * Tetroguer * Tetropil * UN 1897 (DOT)
	*
131-11-3	Dimethyl phthalate * <u>1,2-Benzenedicarboxylic acid,</u>
	<u>dimethyl ester</u> * Avolin * Dimethyl-1,2-benzenedicarboxylate *
	Dimethyl benzeneorthodicarboxylate * Dimethyl ester 1,2-
	benzenedicarboxylic acid * o-Dimethylphthalate * Dimethyl-o-
	phthalate * DMP * ENT 262 * Fermin * Methyl phthalate *
	Mipax * NTM * Palatinol M * Phthalic acid, dimethyl ester *
	Phthalic acid, methyl ester * RCRA Waste Number U102 *
	Repeftal * Solvanom * Solvarone * Unimoll DM *
143-33-9	<u>Sodium cyanide</u> * Cyanide of sodium * Cyanogran * Cymag *
	Hydrocyanic acid * Hydrocyanic acid, sodium salt * Sodium
	salt * RCRA Waste Number P106 * UN 1689 (DOT) *



151-50-8	<u>Potassium cyanide</u> * Cyanide of potassium * Hydrocyanic acid * Hydrocyanic acid, potassium salt * Potassium salt * RCRA Waste Number P098 * UN 1680 (DOT) *
156-60-5	<i>trans</i> -1,2-Dichloroethene * <u>Ethene, 1,2-dichloro-, (E)-</u> * <i>trans</i> -Acetylene dichloride * 1,2-Dichloroethene * (E)-1,2-Dichloroethene * Dichloroethylene * 1,2-Dichloroethylene * <i>trans</i> -Dichloroethylene * <i>trans</i> -1,2-Dichloroethylene * Dioform * RCRA Waste Number U079 *
205-99-2	<u>Benz(e)acephenanthrylene</u> * BbFL * BbF * 3,4-Benz(e)acephenanthrylene * 2,3-Benzfluoranthene * 3,4-Benzfluoranthene * Benzo(b)fluoranthene * Benzo(e)fluoranthene * 2,3-Benzofluoranthene * 3,4-Benzofluoranthene * 2,3-Benzofluoranthrene * B(b)F *
206-44-0	<u>Fluoranthene</u> * 1,2-Benzacenaphthene * Benzo(jk)fluorene * Idryl * 1,2-(1,8-Naphthylene)benzene * 1,2-(1,8-Naphthalenediyl)benzene * RCRA Waste Number U120 *
218-01-9	<u>Chrysene</u> * 1,2-Benzophenanthrene * Benzo(a)phenanthrene * 1,2-Benzphenanthrene * Benz(a)phenanthrene * CH * CR * 1,2,5,6-Dibenzonaphthalene * RCRA Waste Number U050 *
309-00-2	Aldrin * <u>1,4:5,8-dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1<math>\alpha</math>,4<math>\alpha</math>,4a<math>\beta</math>,5<math>\alpha</math>,8<math>\alpha</math>,8a<math>\beta</math>)-</u> * Aldocit * Aldrec * Aldrex * Aldrex 30 * Aldrite * Aldrosol * Compound 118 * Drinox * ENT 15949 * 1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, <i>endo</i> , <i>exo</i> - * Hexachlorohexahydro- <i>endo</i> , <i>exo</i> -dimethanonaphthalene * 1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimethanonaphthalene * 1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro- <i>exo</i> -1,4- <i>endo</i> -5,8-dimethanonaphthalene * 1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-1,4- <i>endo</i> - <i>exo</i> -5,8-dimethanonaphthalene * HHDN * Kortofin * NA 2761 * NA 2762 * NCI-C00044 * Octalene * RCRA Waste Number P004 * SD 2794 * Seedrin * Seedrin liquid * Tatuzinno * Tipula *
541-73-1	1,3-Dichlorobenzene * <u>Benzene, 1,3-dichloro-</u> * <i>m</i> -Dichlorobenzene * <i>m</i> -Dichlorobenzol * Metadichlorobenzene * <i>m</i> -Phenylene dichloride * RCRA Waste Number U071 * UN 1591 (DOT) *
542-88-1	<i>Bis</i> (chloromethyl) ether * <u>Methane, oxybis[chloro-</u> * BCME * Chloro(chloromethoxy) methane * Chloromethyl ether * Dichlorodimethylether * $\alpha$ , $\alpha'$ -Dichlorodimethyl ether * <i>sym</i> -Dichloro-dimethyl ether * <i>sym</i> -Dichloromethyl ether * Dichloromethyl ether * Dimethyl-1,1'-dichloroether * Monochloromethyl ether * Oxybis(chloromethane) *
606-20-2	2,6-Dinitrotoluene * <u>Benzene, 2-methyl-1,3-dinitro-</u> * 2,6-DNT * 2-methyl-1,3-dinitrobenzene * RCRA Waste Number U106 *
1746-01-6	Dioxins (TCDD) * <u>Dibenzo[b,e][1,4]dioxin, 2,3,7,8-tetrachloro-</u> * Dioxin * Dioxin (herbicide contaminant) * Dioxine * NCI-C03714 * TCDBD * TCDD * 2,3,7,8-TCDD * 2,3,7,8-Tetrachloro-dibenzo(b,e)(1,4)dioxan * 2,3,7,8-Tetrachloro-dibenzo- <i>p</i> -doixin * 2,3,7,8-Tetrachloro-dibenzo-1,4-dioxin * Tetradoxin *
7439-92-1	<u>Lead</u> * Pb * C.I. 77575 * C.I. Pigment metal 4 * Glover * KS-4 * Lead flake * Lead S2 * Lead SO * Omaha * Omaha & Grant * SO * S1 *

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7439-97-6	<u>Mercury</u> * Hg * Colloidal mercury * Metallic mercury * NA 2809 (DOT) * NCI-C60399 * Quicksilver * RCRA Waste Number U151 * UN 2809 (DOT) *
7440-02-0	<u>Nickel</u> * Ni * Carbonyl nickel powder * C.I. 77775 * NI 270 * Nickel 270 * Nickel (dust) * Nickel particles * Nickel sponge * NI 0901-S * NI 4303T * NP 2 * Raney alloy * Raney nickel *
7440-22-4	<u>Silver</u> * Ag * Argentum * C.I. 77820 * L 3 * Shell silver * Silflake 135 * Silver atom * Silver metal * Sr 999 * V 9 *
7440-28-0	<u>Thallium</u> * Tl * Ramor *
7440-38-2	<u>Arsenic</u> * Arsenicals * Arsenic-75 * Arsenic black * colloidal arsenic * Grey arsenic * Metallic arsenic * UN 1558 (DOT) *
7440-41-7	<u>Beryllium</u> * Be * Beryllium-9 * Glucinium * Glucinum * RCRA Waste Number P015 * UN 1567 (DOT) *
7440-43-9	<u>Cadmium</u> * Cd * C.I. 77180 * colloidal cadmium *
7440-47-3	<u>Chromium</u> * Chrome * Cr *
7440-50-8	<u>Copper</u> * Cu * Allbri natural copper * Anac 110 * Arwood copper * Bronze powder * CDA 101 * CDA 102 * CDA 110 * CDA 122 * C.I. 77400 * C.I. Pigment metal 2 * Copper-airborne * Copper bronze * Copper M 1 * Copper-milled * Copper powder * Copper slag-airborne * Copper slag-milled * CuEP * CuEPP * Cu M2 * Cu M3 * DCuPl * E-Copper * E-Cu57 * E-Cu F20GB * 1721 Gold * Gold bronze * Kafar copper * M 1 * M 3 * M 4 * M1 (copper) * M2 (copper) * M3 (copper) * M4 (copper) * M3R * M3S * OFHC Cu * Raney copper *
7440-66-6	<u>Zinc</u> * Zn * Asarco L 15 * Blue powder * C.I. 77945 * C.I. Pigment black 16 * C.I. Pigment metal 6 * Emanay zinc dust * Granular zinc * Jasad * Merrillite * Non-pyrophoric zinc * Pasco * Pyrophoric zinc * UN 1383 (DOT) * UN 1436 (DOT) * Zinc dust * Zinc powder *
7664-41-7	<u>Ammonia</u> * Am-fol * Ammonia gas * Anhydrous ammonia * Liquid ammonia * Nitro-Sil * R 717 * Spirit of Hartshorn * UN 1005 (DOT) * UN 2073 (DOT) *
7732-18-5	<u>Water</u> * Dihydrogen oxide * Distilled water * Ice * Water vapor *
7782-49-2	<u>Selenium</u> * Se * C.I. 77805 * Colloidal selenium * Elemental selenium * Non-pyrophoric selenium metal powder * Selen (polish) * Selenate * Selenium alloy * Selenium base * Selenium dust * Selenium Homopolymer * UN 2658 (DOT) * Vandex *
8001-35-2	<u>Toxaphene</u> * Agricide maggot killer (F) * Alltex * Alltox * Anatox * Attac 4-2 * Attac 4-4 * Attac 6 * Attac 6-3 * Attac 8 * Camphechlor * Camphochlor * Chem-phene M5055 * Chlor chem T-590 * Chlorinated camphene * Chlorocamphene * Compound 3956 * Crestoxo * Crestoxo 90 * ENT 9735 * Estonox * Fasco-terpene * Geniphene * Gy-phene * Hercules 3956 * Hercules Motox * Hercules toxaphene * Huilex * Kamfachlor * M 5055 * Melipax * Motox * NA 2761 * NCI-C00259 * Octachlorocamphene * PCC * PChK * Penphene * Phenacide * Phenatox * Phenphane * Polychlorcamphene * Polychlorinated camphenes * Polychlorocamphene * RCRA Waste Number P123 * Synthetic 3956 * Strobane-T * Strobane-T90 * Texadust * Toxakil * Toxaphen * Toxon 63 * Toxyphen * Vertac 90% * Vertac toxaphene 90*

11096-82-5      Aroclor 1260 \* Chlorodiphenyl (60% Cl) \* Chlorphen A60 \*  
 Kanechlor \* PCB-1260 \* Phenochlor DP6 \* Polychlorinated  
 biphenyl \* Polychlorobiphenol \* UN 2315 (DOT) \*

## 36 - Table 4

Table 4. The selected 108 substances ordered by number of carbon and hydrogen atoms. The Chemical Abstracts Service Registry Numbers (CAS RN) are noted. Inorganic chemicals and elements appear at the end.

<u>Formula</u>	<u>CAS RN</u>	<u>Substance</u>
CCl <sub>2</sub> F <sub>2</sub>	75-71-8	Dichlorodifluoromethane
CCl <sub>3</sub> F	75-69-4	Trichlorofluoromethane
CCl <sub>4</sub>	56-23-5	Carbon tetrachloride
CNK	151-50-8	Potassium cyanide
CNNa	143-33-9	Sodium cyanide
CS <sub>2</sub>	75-15-0	Carbon disulfide
CHBr <sub>2</sub> Cl	124-48-1	Dibromochloromethane
CHBr <sub>3</sub>	75-25-2	Bromoform
CHCl <sub>3</sub>	67-66-3	Chloroform
CHN	74-90-8	Hydrogen cyanide
CH <sub>2</sub> Cl <sub>2</sub>	75-09-2	Dichloromethane
CH <sub>3</sub> Br	74-83-9	Bromomethane
CH <sub>3</sub> Cl	74-87-3	Chloromethane
CH <sub>4</sub> O	67-56-1	Methanol
C <sub>2</sub> Cl <sub>4</sub>	127-18-4	Tetrachloroethene
C <sub>2</sub> Cl <sub>6</sub>	67-72-1	Hexachloroethane
C <sub>2</sub> HCl <sub>3</sub>	79-01-6	Trichloroethene
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	75-35-4	1,1-Dichloroethene
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	156-60-5	<i>trans</i> -1,2-Dichloroethene
C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub>	79-34-5	1,1,2,2-Tetrachloroethane
C <sub>2</sub> H <sub>3</sub> Cl	75-01-4	Vinyl chloride
C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	71-55-6	1,1,1-Trichloroethane
C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	79-00-5	1,1,2-Trichloroethane
C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub>	106-93-4	1,2-Dibromomethane
C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	75-34-3	1,1-Dichloroethane
C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	107-06-2	1,2-Dichloroethane
C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub> O	542-88-1	<i>Bis</i> (chloromethyl)ether
C <sub>2</sub> H <sub>4</sub> O	75-21-8	Ethylene oxide
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	64-19-7	Acetic acid
C <sub>2</sub> H <sub>5</sub> Cl	75-00-3	Chloroethane
C <sub>2</sub> H <sub>6</sub> O	64-17-5	Ethanol
C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	107-21-1	Ethylene glycol
C <sub>2</sub> H <sub>6</sub> OS	67-68-5	Dimethyl sulfoxide
C <sub>3</sub> H <sub>3</sub> N	107-13-1	Acrylonitrile
C <sub>3</sub> H <sub>4</sub> O	107-02-8	Acrolein
C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub>	78-87-5	1,2-Dichloropropane
C <sub>3</sub> H <sub>6</sub> O	67-64-1	Acetone
C <sub>4</sub> Cl <sub>6</sub>	87-68-3	Hexachlorobutadiene
C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> O	111-44-4	<i>Bis</i> (2-chloroethyl)ether
C <sub>4</sub> H <sub>8</sub> O	78-93-3	2-Butanone
C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	123-91-1	1,4-Dioxane
C <sub>6</sub> Cl <sub>6</sub>	118-74-1	Hexachlorobenzene
C <sub>6</sub> HCl <sub>5</sub> O	87-86-5	Pentachlorophenol
C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub>	120-82-1	1,2,4-Trichlorobenzene
C <sub>6</sub> H <sub>3</sub> Cl <sub>3</sub> O	88-06-2	2,4,6-Trichlorophenol
C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	95-50-1	1,2-Dichlorobenzene
C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	541-73-1	1,3-Dichlorobenzene
C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	106-46-7	1,4-Dichlorobenzene

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<u>Formula</u>	<u>CAS RN</u>	<u>Substance</u>
C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> O	120-83-2	2,4-Dichlorophenol
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>5</sub>	51-28-5	2,4-Dinitrophenol
C <sub>6</sub> H <sub>5</sub> Cl	108-90-7	Chlorobenzene
C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	98-95-3	Nitrobenzene
C <sub>6</sub> H <sub>6</sub>	71-43-2	Benzene
C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub>	58-89-9	γ-Hexachlorocyclohexane (Lindane)
C <sub>6</sub> H <sub>6</sub> O	108-95-2	Phenol
C <sub>6</sub> H <sub>7</sub> N	62-53-3	Aniline
C <sub>6</sub> H <sub>12</sub>	110-82-7	Cyclohexane
C <sub>6</sub> H <sub>12</sub> O	108-10-1	4-Methyl-2-pentanone
C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	121-14-2	2,4-Dinitrotoluene
C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	606-20-2	2,6-Dinitrotoluene
C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	65-85-0	Benzoic acid
C <sub>7</sub> H <sub>7</sub> ClO	59-50-7	6-Chloro- <i>m</i> -cresol
C <sub>7</sub> H <sub>8</sub>	108-88-3	Toluene
C <sub>7</sub> H <sub>8</sub> O	95-48-7	<i>o</i> -Cresol
C <sub>8</sub> H <sub>10</sub>	100-41-4	Ethylbenzene
C <sub>8</sub> H <sub>10</sub>	108-38-3	<i>m</i> -Xylene
C <sub>8</sub> H <sub>10</sub>	95-47-6	<i>o</i> -Xylene
C <sub>8</sub> H <sub>10</sub>	106-42-3	<i>p</i> -Xylene
C <sub>8</sub> H <sub>10</sub> O	105-67-9	2,4-Xylenol
C <sub>9</sub> H <sub>7</sub> N	91-22-5	Quinoline
C <sub>9</sub> H <sub>14</sub> O	78-59-1	Isophorone
C <sub>10</sub> H <sub>5</sub> Cl <sub>7</sub>	76-44-8	Heptachlor
C <sub>10</sub> H <sub>6</sub> Cl <sub>8</sub>	57-74-9	Chlordane
C <sub>10</sub> H <sub>8</sub>	91-20-3	Naphthalene
C <sub>10</sub> C <sub>10</sub> Cl <sub>8</sub>	8001-35-2	Toxaphene
C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	131-11-3	Dimethyl phthalate
C <sub>12</sub> H <sub>4</sub> Cl <sub>4</sub> O <sub>2</sub>	1746-01-6	Dioxins (TCDD)
C <sub>12</sub> H <sub>8</sub> Cl <sub>6</sub>	309-00-2	Aldrin
C <sub>12</sub> H <sub>8</sub> Cl <sub>6</sub> O	60-57-1	Dieldrin
C <sub>12</sub> H <sub>8</sub> Cl <sub>6</sub> O	72-20-8	Endrin
(C <sub>12</sub> H <sub>10-x</sub> )Cl <sub>x</sub>	11096-82-5	Aroclor 1260 (PCB 1260)
C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O	86-30-6	N-Nitrosodiphenylamine
C <sub>12</sub> H <sub>12</sub> N <sub>2</sub>	92-87-5	Benzidine
C <sub>12</sub> H <sub>14</sub> O <sub>4</sub>	84-66-2	Diethyl phthalate
C <sub>14</sub> H <sub>9</sub> Cl <sub>5</sub>	50-29-3	DDT
C <sub>14</sub> H <sub>10</sub>	85-01-8	Phenanthrene
C <sub>16</sub> H <sub>10</sub>	206-44-0	Fluoranthene
C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	84-74-2	Dibutyl phthalate
C <sub>18</sub> H <sub>12</sub>	56-55-3	Benz[ <i>a</i> ]anthracene
C <sub>18</sub> H <sub>12</sub>	218-01-9	Chrysene
C <sub>20</sub> H <sub>12</sub>	205-99-2	Benz( <i>e</i> )acephenanthrylene
C <sub>20</sub> H <sub>12</sub>	50-32-8	Benzo[ <i>a</i> ]pyrene
C <sub>22</sub> H <sub>14</sub>	53-70-3	Dibenz[ <i>a,h</i> ]anthracene
C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>	117-81-7	Bis(2-ethylhexyl)phthalate
Ag	7440-22-4	Silver
As	7440-38-2	Arsenic
Be	7440-41-7	Beryllium
Cd	7440-43-9	Cadmium
Cr	7440-47-3	Chromium
Cu	7440-50-8	Copper

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<u>Formula</u>	<u>CAS RN</u>	<u>Substance</u>
H <sub>2</sub> O	7732-18-5	Water
NH <sub>3</sub>	7664-41-7	Ammonia
Hg	7439-97-6	Mercury
Ni	7440-02-0	Nickel
Pb	7439-92-1	Lead
Se	7782-49-2	Selenium
Tl	7440-28-0	Thallium
Zn	7440-66-6	Zinc

**Table 5.** Ranking of the 108 selected substances by specific gravity at 20/4 (i.e. the ratio of the density of the substance at 20°C to that of water at 4°C) unless otherwise noted. Values less than 1.0 indicate hydrophobic substances will float on water. Hydrophilic substances, for example acetone, are miscible with water and do not float or sink. Common components in gasoline and other hydrocarbon fuels are noted with an asterisk (\*) before the name.

<u>Substance</u>	<u>CAS RN</u>	<u>Specific Gravity</u>	
Hydrogen Cyanide	74-90-8	0.688	
Ammonia	7664-41-7	0.7188 g/L gas	
Cyclohexane	110-82-7	0.77855	
*Ethanol	64-17-5	0.7893	
Acetone	67-64-1	0.7900	
*Methanol	67-56-1	0.7914	
4-Methyl-2-pentanone	108-10-1	0.8010	
2-Butanone	78-93-3	0.8049	
Acrylonitrile	107-13-1	0.8060	
Acrolein	107-02-8	0.8389	
*p-Xylene	106-42-3	0.8611	
*m-Xylene	108-38-3	0.86436	
*Toluene	108-88-3	0.86683	
*Ethylbenzene	100-41-4	0.8670	
Ethylene oxide	75-21-8	0.8694	
*Benzene	71-43-2	0.8790	
*o-Xylene	95-47-6	0.8802	
Chloroethane	75-00-3	0.8960	
Vinyl chloride	75-01-4	0.9106	
Chloromethane	74-87-3	0.9214	
Isophorone	78-59-1	0.9229	Δ
2,4-Xylenol	105-67-9	0.9650	
Bis(2-ethylhexyl)phthalate	117-81-7	0.9843	floaters
Water	7732-18-5	1.0000	
Aniline	62-53-3	1.0217	sinkers
*Phenanthrene	85-01-8	1.025	
Naphthalene	91-20-3	1.0253	▽
*o-Cresol	95-48-7	1.02734	
1,4-Dioxane	123-91-1	1.03361	
Dibutyl phthalate	84-74-2	1.0465	
Acetic acid	64-19-7	1.04955	
*Phenol	108-95-2	1.070	
Quinoline	91-22-5	1.0929	
Dimethyl sulfoxide	67-68-5	1.10041	
Chlorobenzene	108-90-7	1.1063	
Ethylene glycol	107-21-1	1.1135	
Diethyl phthalate	84-66-2	1.1175	
1,2-Dichloropropane	78-87-5	1.15597	
*1,1-Dichloroethane	75-34-3	1.1755	
Dimethyl phthalate	131-11-3	1.2	
Nitrobenzene	98-95-3	1.20331	
1,1-Dichloroethene	75-35-4	1.213229	
6-Chloro-m-cresol	59-50-7	1.215 @ 15°C	

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<u>Substance</u>	<u>CAS RN</u>	<u>Specific Gravity</u>
Bis(2-chloroethyl)ether	111-44-4	1.2192
N-Nitrosodiphenylamine	86-30-6	1.23
*1,2-Dichloroethane	107-06-2	1.2351
1,4-Dichlorobenzene	106-46-7	1.2475
Benzidine	92-87-5	1.250
*Fluoranthene	206-44-0	1.252 @ 0/4
trans-1,2-Dichloroethene	156-60-5	1.2547
*Carbon disulfide	75-15-0	1.26311
Benzoic acid	65-85-0	1.27
*Benz[a]anthracene	56-55-3	1.274
*Chrysene	218-01-9	1.274
*Dibenz[a,h]anthracene	53-70-3	1.282
2,6-Dinitrotoluene	606-20-2	1.2833 @ 111°C
1,3-Dichlorobenzene	541-73-1	1.28844
Aroclor 1260 (PCB 1260)	11096-82-5	1.3-1.8
1,2-Dichlorobenzene	95-50-1	1.3048
Bis(chloromethyl)ether	542-88-1	1.315
Dichloromethane	75-09-2	1.3256
Dichlorodifluoromethane	75-71-8	1.3292
1,1,1-Trichloroethane	71-55-6	1.3381
Benzo[a]pyrene	50-32-8	1.351
2,4-Dichlorophenol	120-83-2	1.4 @ 15°C
1,1,2-Trichloroethane	79-00-5	1.43931
1,2,4-Trichlorobenzene	120-82-1	1.45420
Trichloroethene	79-01-6	1.4642
Trichlorofluoromethane	75-69-4	1.467 @ 25°C
Chloroform	67-66-3	1.49
Potassium cyanide	151-50-8	1.52 @ 16°C
2,4-Dinitrotoluene	121-14-2	1.521 @ 15°C
Hexachlorobutadiene	87-68-3	1.5542
DDT	50-29-3	1.56 @ 15°C
Hexachlorobenzene	118-74-1	1.5691 @ 23.6°C
Carbon tetrachloride	56-23-5	1.59402
1,1,2,2-Tetrachloroethane	79-34-5	1.59449
Aldrin	309-00-2	1.6
Chlordane	57-74-9	1.6
Sodium cyanide	143-33-9	1.60 @ 25°C
Tetrachloroethene	127-18-4	1.6227
Toxaphene	8001-35-2	1.63
Heptachlor	76-44-8	1.66
2,4,6-Trichlorophenol	88-06-2	1.675
Bromomethane	74-83-9	1.6758
2,4-Dinitrophenol	51-28-5	1.68
Endrin	72-20-8	1.7
Dieldrin	60-57-1	1.75
Beryllium	7440-41-7	1.8477
γ-Hexachlorocyclohexane (Lindane)	58-89-9	1.89
Pentachlorophenol	87-86-5	1.978
Hexachloroethane	67-72-1	2.091
1,2-Dibromoethane	106-93-4	2.1792
Dibromochloromethane	124-48-1	2.451
Bromoform	75-25-2	2.8899



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<u>Substance</u>	<u>CAS RN</u>	<u>Specific Gravity</u>
Selenium	7782-49-2	4.81
Arsenic	7440-38-2	5.72
Zinc	7440-66-6	7.14
Chromium	7440-47-3	7.18-7.20
Cadmium	7440-43-9	8.642
Nickel	7440-02-0	8.908
Copper	7440-50-8	8.94
Silver	7440-22-4	10.50
*Lead	7439-92-1	11.35
Thallium	7440-28-0	11.85
103 Mercury	7439-97-6	13.5939
*Benz(e)acephenanthrylene	205-99-2	unknown
Dioxins (TCDD)	1746-01-6	unknown

## 42 - Table 6

**Table 6.** Solubilities of the 108 selected hazardous substances in various solvents. Values when given are in weight percents (wt%). All values are for solutions at room temperatures (approximately 15°C to 25°C) except as noted. Abbreviations are:

M	miscible	100%
V	very soluble	> 50%
So	soluble	5-50%
Sl	slightly soluble	< 5%
I	insoluble	0% (or <0.001%)
-	unknown	
decom.	decomposes	
ethan	ethanol	
acet	acetone	
benz	benzene	

<u>Substance</u>	<u>CAS RN</u>	<u>Water</u>	<u>Ethan</u>	<u>Acet</u>	<u>Benz</u>	<u>Ether</u>
Acetic acid	64-19-7	M	M	M	M	M
Acetone	67-64-1	M	M	M	M	M
Acrolein	107-02-8	20.8	So	So	So	So
Acrylonitrile	107-13-1	7.35	M	So	So	M
Aldrin	309-00-2	I	So	So	So	So
Ammonia	7664-41-7	53.1	21@0°C	So	So	So
Aniline	62-53-3	3.38	M	M	M	M
Aroclor 1260 (PCB 1260)	11096-82-5	I	-	-	-	-
Arsenic	7440-38-2	I	-	-	-	-
Benz(e)acephenanthrylene	205-99-2	I	-	-	Sl	-
Benz[a]anthracene	56-55-3	I	Sl	So	V	So
Benzene	71-43-2	0.179	M	M	M	M
Benzidine	92-87-5	0.052	Sl	-	-	Sl
Benzoic acid	65-85-0	0.29	46.6	So	So	66
Benzo[a]pyrene	50-32-8	0.003	Sl	-	So	-
Beryllium	7440-41-7	I	-	-	-	-
Bis(2-chloroethyl)ether	111-44-4	1.1	So	So	M	So
Bis(chloromethyl)ether	542-88-1	decom.	M	-	-	M
Bis(2-ethylhexyl)phthalate	117-81-7	<0.01	-	-	-	-
Bromoform	75-25-2	0.318	M	-	M	M
Bromomethane	74-83-9	0.09	M	M	M	M
2-Butanone	78-93-3	24	M	M	M	M
Cadmium	7440-43-9	I	-	-	-	-
Carbon disulfide	75-15-0	0.21	M	-	-	M
Carbon tetrachloride	56-23-5	0.08	M	M	M	M
Chlordane	57-74-9	I	M	M	M	M
Chlorobenzene	108-90-7	0.05	M	M	M	M
6-Chloro-m-cresol	59-50-7	0.004	So	So	So	So
Chloroethane	75-00-3	0.57	48.3	-	-	M
Chloroform	67-66-3	0.82	M	So	M	M
Chloromethane	74-87-3	0.48	So	-	M	M
Chromium	7440-47-3	I	-	-	-	-
Chrysene	218-01-9	I	Sl	Sl	Sl	Sl
Copper	7440-50-8	I	-	-	-	-
o-Cresol	95-48-7	Sl	V	M	M	V
Cyclohexane	110-82-7	0.01	M	M	M	M

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<u>Substance</u>	<u>CAS RN</u>	<u>Water</u>	<u>Ethan</u>	<u>Acet</u>	<u>Benz</u>	<u>Ether</u>
DDT	50-29-3	I	S1	58	75	V
Dibenz[ <i>a,h</i> ]anthracene	53-70-3	I	S1	S1	V	I
Dibromochloromethane	124-48-1	I	S	S	S	S
Dibutyl phthalate	84-74-2	0.45	V	V	V	V
1,3-Dichlorobenzene	541-73-1	0.011	S	S	S	S
1,2-Dichlorobenzene	95-50-1	0.015	S	S	S	S
1,4-Dichlorobenzene	106-46-7	0.008	M	M	S1	S1
Dichlorodifluoromethane	75-71-8	0.028	S	-	9	S
1,1-Dichloroethane	75-34-3	0.5	V	S	S	V
1,2-Dichloroethane	107-06-2	0.81	M	S	S	M
1,1-Dichloroethene	75-35-4	0.021	S	S	S	V
<i>trans</i> -1,2-Dichloroethene	156-60-5	0.63	M	M	V	M
Dichloromethane	75-09-2	1.3	M	-	-	M
2,4-Dichlorophenol	120-83-2	0.45	So	-	S	So
1,2-Dichloropropane	78-87-5	0.274	S	-	S	S
Dieldrin	60-57-1	I	S1	S	S	-
Diethyl phthalate	84-66-2	0.021	M	S	S	M
Dimethyl phthalate	131-11-3	0.5	M	-	M	M
Dimethyl sulfoxide	67-68-5	25.3	S	S	S	S
2,4-Dinitrophenol	51-28-5	0.56	S	35.9	S	S
2,4-Dinitrotoluene	121-14-2	0.03	1.2	S	S	9
2,6-Dinitrotoluene	606-20-2	-	S	-	-	-
1,4-Dioxane	123-91-1	M	M	M	M	M
Dioxins (TCDD)	1746-01-6	I	-	-	-	-
Endrin	72-20-8	I	-	17	13.8	-
Ethanol	64-17-5	M	M	M	So	M
Ethylbenzene	100-41-4	0.015	S	-	M	V
1,2-Dibromoethane	106-93-4	0.429	M	S	S	M
Ethylene glycol	107-21-1	M	V	V	S1	1.0
Ethylene oxide	75-21-8	M	M	S	S	V
Fluoranthene	206-44-0	I	S	-	S	S
Heptachlor	76-44-8	I	S	-	S	S
Hexachlorobenzene	118-74-1	I	S	-	S	S
Hexachlorobutadiene	87-68-3	I	S	S	-	S
$\gamma$ -Hexachlorocyclohexane (Lindane)	58-89-9	0.001	6.4	44.5	28.9	20.8
Hexachloroethane	67-72-1	0.005	V	-	S	V
Hydrogen cyanide	74-90-8	M	M	-	-	So
Isophorone	78-59-1	1.2	S	S	-	S
Lead	7439-92-1	I	-	-	-	-
Mercury	7439-97-6	I	I	-	-	I
Methanol	67-56-1	M	M	M	M	M
4-Methyl-2-pentanone	108-10-1	1.7	M	M	M	M
Naphthalene	91-20-3	0.003	7.0	V	33.0	V
Nickel	7440-02-0	I	-	-	-	-
Nitrobenzene	98-95-3	0.19	V	V	M	M
N-Nitrosodiphenylamine	86-30-6	I	S1	S	S	-
Pentachlorophenol	87-86-5	0.002	V	-	S	S
Phenanthrene	85-01-8	I	S	S	50	30
Phenol	108-95-2	8.66	V	-	8.2	V
Potassium cyanide	151-50-8	71.6	S1	-	-	-
Quinoline	91-22-5	0.6	M	M	M	M
Selenium	7782-49-2	I	-	-	-	-

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<u>Substance</u>	<u>CAS RN</u>	<u>Water</u>	<u>Ethan</u>	<u>Acet</u>	<u>Benz</u>	<u>Ether</u>
Silver	7440-22-4	I	-	-	-	-
Sodium cyanide	143-33-9	58	So	-	-	-
1,1,2,2-Tetrachloroethane	79-34-5	0.29	M	S	S	M
Tetrachloroethene	127-18-4	0.015	M	-	M	M
Thallium	7440-28-0	I	-	-	-	-
Toluene	108-88-3	0.05	M	S	M	M
Toxaphene	8001-35-2	I	-	-	-	-
1,2,4-Trichlorobenzene	120-82-1	I	Sl	-	M	M
1,1,1-Trichloroethane	71-55-6	0.132	M	S	S	M
1,1,2-Trichloroethane	79-00-5	0.44	M	-	-	M
Trichloroethene	79-01-6	0.137	M	S	-	M
Trichlorofluoromethane	75-69-4	0.11	M	-	-	M
2,4,6-Trichlorophenol	88-06-2	0.8	V	V	-	V
Vinyl chloride	75-01-4	0.27	S	-	S	V
Water	7732-18-5	M	M	-	M	-
<i>m</i> -Xylene	108-38-3	0.02	M	M	M	M
<i>o</i> -Xylene	95-47-6	0.017	M	M	M	M
<i>p</i> -Xylene	106-42-3	0.016	M	M	M	M
2,4-Xylenol	105-67-9	0.787	M	-	S	M
Zinc	7440-66-6	I	-	-	-	-

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Table 7. The 108 selected substances ordered by vapor pressure (in kPa) at 20°C unless noted otherwise. Values less than  $10^{-5}$  are assigned zero. Unknown means no values were found in the literature. Chemical Abstracts Service Registry Numbers (CAS RN), boiling points (BP), and vapor pressures in mm Hg are noted also. Vapor pressure is a good indicator of the volatility of a substance and its detectability with gas sniffers.

Substance	CAS RN	Vapor Pressure		BP (°C)
		kPa	(mm Hg)	
Ammonia	7664-41-7	881.53	(6612)	-33.42
Dichlorodifluoromethane	75-71-8	566.62	(4250)	-29.8
Chloromethane	74-87-3	506.6	(3800)	-24.2
Vinyl chloride	75-01-4	306.6	(2300)	-13.9
Bromomethane	74-83-9	166.6	(1250)	3.56
Ethylene oxide	75-21-8	146.0	(1095)	10.7
Chloroethane	75-00-3	133.32	(1000)	12.27
Trichlorofluoromethane	75-69-4	91.598	(687)	23.8
Hydrogen cyanide	74-90-8	82.6	(620)	25.7
1,1-Dichloroethene	75-35-4	66.661	(500)	32
Dichloromethane	75-09-2	46.53	(349)	40
<i>trans</i> -1,2-Dichloroethene	156-60-5	35.33	(265)	47.7
Carbon disulfide	75-15-0	34.664	(260)	46.25
Acrolein	107-02-8	29.33	(220)	52.5
Acetone	67-64-1	24.227	(181.7)	56.2
1,1-Dichloroethane	75-34-3	23.998	(180)	57.28
Chloroform	67-66-3	21.33	(160)	61.2
1,1,1-Trichloroethane	71-55-6	13.33	(100)	74.1
Methanol	67-56-1	12.27	(92)	64.7
Carbon tetrachloride	56-23-5	12.0	(90)	76.54
Acrylonitrile	107-13-1	11.0	(83)	77.4
2-Butanone	78-93-3	10.333	(77.5)	79.58
Cyclohexane	110-82-7	10.3	(77)	80.74
Benzene	71-43-2	10.13	(76)	80.1
Dibromochloromethane	124-48-1	10.13	(76)	118.
1,2-Dichloroethane	107-06-2	8.13	(61)	83.47
Trichloroethene	79-01-6	8.0	(60)	86.7
1,2-Dichloropropane	78-87-5	5.60	(42)	96.37
Ethanol	64-17-5	5.333	(40) @ 19°C	78.293
1,4-Dioxane	123-91-1	4.00	(30)	101.3
<i>Bis</i> (chloromethyl) ether	542-88-1	4.00	(30) @ 22°C	105
Toluene	108-88-3	2.93	(22)	110.6
1,1,2-Trichloroethane	79-00-5	2.533	(19)	113.7
Water	7732-18-5	2.3378	(17.53)	100
4-Methyl-2-pentanone	108-10-1	2.13	(16)	116.85
Tetrachloroethene	127-18-4	1.87	(14)	121
Acetic acid	64-19-7	1.520	(11.4)	117.9
1,2-Dibromoethane	106-93-4	1.467	(11)	131.36
Benzidine	92-87-5	1.333	(10) @ 30°C	402
Chlorobenzene	108-90-7	1.17	(8.8)	131.7
Ethylbenzene	100-41-4	0.947	(7.1)	136.2
<i>p</i> -Xylene	106-42-3	0.866	(6.5)	138.35
<i>m</i> -Xylene	108-38-3	0.800	(6)	139.1
Bromoform	75-25-2	0.667	(5)	149.5

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Substance	CAS RN	Vapor Pressure		BP (°C)
		kPa	(mm Hg)	
1,1,2,2-Tetrachloroethane	79-34-5	0.666	(5)	146.2
o-Xylene	95-47-6	0.666	(5)	144.4
1,3-Dichlorobenzene	541-73-1	0.252	(1.89) @ 25°	173
Thallium	7440-28-0	0.133	(1) @ 825°C	1457
Zinc	7440-66-6	0.133	(1) @ 487°C	419.58
Arsenic	7440-38-2	0.133	(1) @ 372°C	613
Copper	7440-50-8	0.133	(1) @ 1628°C	2567
Beryllium	7440-41-7	0.133	(1) @ 1520°C	2970
Phenanthrene	85-01-8	0.133	(1) @ 118.3°C	340
Lead	7439-92-1	0.133	(1)	970
1,2-Dichlorobenzene	95-50-1	0.133	(1)	180.5
Bis(2-chloroethyl)ether	111-44-4	0.095	(0.71)	178
1,4-Dichlorobenzene	106-46-7	0.080	(0.6)	174
Hexachloroethane	67-72-1	0.0533	(0.4)	186.8
Dimethyl sulfoxide	67-68-5	0.0493	(0.369)	189
o-Cresol	95-48-7	0.041	(0.31) @ 25°C	190.95
Aniline	62-53-3	0.04	(0.3)	184.13
1,2,4-Trichlorobenzene	120-82-1	0.0388	(0.29) @ 25°C	213
Toxaphene	8001-35-2	0.027-.053	(0.2-.04)	Decomposes
Phenol	108-95-2	0.027	(0.2)	181.8
Isophorone	78-59-1	0.0267	(0.2)	215.2
Hexachlorobutadiene	87-68-3	0.020	(0.15) @ 25°C	215
Nitrobenzene	98-95-3	0.020	(0.15)	210.8
2,4-Dichlorophenol	120-83-2	0.016	(0.12)	210
2,4-Xylenol	105-67-9	0.013	(0.098) @ 25°C	27
Quinoline	91-22-5	0.0112	(0.084) @25°C	238
Ethylene glycol	107-21-1	0.0067	(0.05)	197.5
Naphthalene	91-20-3	0.0067	(0.05)	218
6-Chloro-m-cresol	59-50-7	0.0067	(0.05)	235
Diethyl phthalate	84-66-2	0.0067	(0.05) @ 70°C	298
Fluoranthene	206-44-0	0.0013	(0.01)	375
Dimethyl phthalate	131-11-3	<0.0013	(0.01)	283.8
Dibutyl phthalate	84-74-2	<0.0013	(0.01)	340
2,4,6-Trichlorophenol	88-06-2	0.0011	(0.008) @24°C	246
2,4-Dinitrotoluene	121-14-2	0.00068	(0.0051)	270
Benzoic acid	65-85-0	0.0006	(0.0045)	249
Mercury	7439-97-6	0.00026	(0.0012)	356.58
Selenium	7782-49-2	0.00013	(0.001)	685
2,4-Dinitrophenol	51-28-5	5.2x10 <sup>-5</sup>	(0.00039mm)	Sublimes
Heptachlor	76-44-8	4.x10 <sup>-5</sup>	(0.0003)	Decomposes
Pentachlorophenol	87-86-5	1.47x10 <sup>-5</sup>	(0.0001)	310
Aldrin	309-00-2	0.		145
DDT	50-29-3	0.		260
Hexachlorobenzene	118-74-1	0.		322
γ-Hexachlorocyclohexane(Lindane)	58-89-9	0.		323.4
Aroclor 1260 (PCB 1260)	11096-82-5	0.		340
Bis(2-ethylhexyl)phthalate	117-81-7	0.		385
Benz[a]anthracene	56-55-3	0.		400
Chrysene	218-01-9	0.		448
Benz(e)acephenanthrylene	205-99-2	0.		481
Benzo[a]pyrene	50-32-8	0.		495

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<u>Substance</u>	<u>CAS RN</u>	<u>Vapor Pressure</u>		<u>BP (°C)</u>
		<u>kPa</u>	<u>(mm Hg)</u>	
Dioxins (TCDD)	1746-01-6	0.		500
Dibenz[a,h]anthracene	53-70-3	0.		524
Cadmium	7440-43-9	0.		765
Sodium cyanide	143-33-9	0.		1496
Potassium cyanide	151-50-8	0.		1625
Silver	7440-22-4	0.		2212
Chromium	7440-47-3	0.		2672
Nickel	7440-02-0	0.		2732
2,6-Dinitrotoluene	606-20-2	0.		Decomposes
Dieldrin	60-57-1	0.		Decomposes
Chlordane	57-74-9	0.		Decomposes
Endrin	72-20-8	0.		Decomposes
N-Nitrosodiphenylamine	86-30-6	unknown		Unknown

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Table 8. Ranking of the selected 108 substances by relative dielectric permittivity (dielectric constant) at room temperature (20°C) unless otherwise noted. The frequency at which the relative permittivity was measured is given if noted in the literature. Relative permittivity is useful in predicting electrical property changes in ground water, soils, etc. in case of a spill or other discharge of a substance. Relative dielectric permittivity is not applicable to metals.

<u>Substance</u>	<u>CAS RN</u>	<u>Relative Dielectric Permittivity</u>
Vacuum	-----	1.000
Cyclohexane	110-82-7	2.023
Dichlorodifluoromethane	75-71-8	2.13 @ 29°C
<i>trans</i> -1,2-Dichloroethene	156-60-5	2.14 @ 25°C
1,4-Dioxane	123-91-1	2.220
Carbon tetrachloride	56-23-5	2.23790
<i>p</i> -Xylene	106-42-3	2.2699
Tetrachloroethene	127-18-4	2.280 @ 25°C
Benzene	71-43-2	2.284
Trichlorofluoromethane	75-69-4	2.303
<i>m</i> -Xylene	108-38-3	2.3742
Toluene	108-88-3	2.376 (10 kHz)
Ethylbenzene	100-41-4	2.4042
1,4-dichlorobenzene	106-46-7	2.41 @ 50°C
<i>o</i> -Xylene	95-47-6	2.568
Hexachlorobutadiene	87-68-3	2.6
Naphthalene	91-20-3	2.62-2.67 @ 21°C
Carbon disulfide	75-15-0	2.643
Phenanthrene	85-01-8	2.8
Trichloroethene	79-01-6	3.42 @ 16°C
Aroclor 1260 (PCB 1260)	11096-82-5	4.3-5.6 @ 25°C
Bromoform	75-25-2	4.39
1,1-Dichloroethene	75-35-4	4.67 @ 16°C
Chloroform	67-66-3	4.806
1,2-Dibromoethane	106-93-4	4.991 @ 22.7°C
1,3-dichlorobenzene	541-73-1	5.04 @ 25°C
<i>Bis</i> (2-ethylhexyl)phthalate	11-78-17	5.3
Acetic acid	64-19-7	6.17
Potassium cyanide	151-50-8	6.2 @??
Vinyl chloride	75-01-4	6.26 @ 17.2°C
Dibutyl phthalate	84-74-2	6.436 @ 30°C
Selenium	7782-49-2	6.6 @ 17-22°C
2,4-Xylenol	105-67-9	6.61 @ 30°C
Chlorobenzene	108-90-7	6.69 (1 MHz)
1,2,4-Trichlorobenzene	120-82-1	6.75 (1.8 MHz)
Aniline	62-53-3	6.89
1,1,2-Trichloroethane	79-00-5	7.29
1,1,1-Trichloroethane	71-55-6	7.52
Dimethyl phthalate	131-11-3	8.5 @ 24°C
1,1,2,2-Tetrachloroethane	79-34-5	8.50 (1.8 MHz)
1,2-Dichloropropane	78-87-5	8.96 @ 25°C
Dichloromethane	75-09-2	9.08
Quinoline	91-22-5	9.12 (3 MHz)



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<u>Substance</u>	<u>CAS RN</u>	<u>Relative Dielectric Permittivity</u>
Chloroethane	75-00-3	9.45
Phenol	108-95-2	9.8 @ 21°C
Bromomethane	74-83-9	9.82 @ 0°C
1,2-dichlorobenzene	95-50-1	9.93 @ 25°C
1,1-Dichloroethane	75-34-3	10.0 @ 18°C
Arsenic	7440-38-2	10.23 (60 MHz)
1,2-Dichloroethane	107-06-2	10.37 @ 25°C
o-Cresol	95-48-7	11.5 @ 25°C
Chloromethane	74-87-3	12.6 @ -20°C
4-Methyl-2-pentanone	108-10-1	13.11
Ethylene oxide	75-21-8	13.9 @ -1°C
Ammonia	7664-41-7	17.8 @ 15°C
2-Butanone	78-93-3	18.51
Acetone	67-64-1	20.9
Bis(2-chloroethyl)ether	111-44-4	21.2
Ethanol	64-17-5	25.07
Acrylonitrile	107-13-1	33.0
Methanol	67-56-1	33.62
Nitrobenzene	98-95-3	35.75 (1.8 MHz)
Ethylene glycol	107-21-1	38.7
Dimethyl sulfoxide	67-68-5	48.9
Water	7732-18-5	80.18
Hydrogen cyanide	74-90-8	114.9
Beryllium	7440-41-7	metal
Cadmium	7440-43-9	metal
Chromium	7440-47-3	metal
Copper	7440-50-8	metal
Lead	7439-92-1	metal
Mercury	7439-97-6	metal
Nickel	7440-02-0	metal
Silver	7440-22-4	metal
Thallium	7440-28-0	metal
Zinc	7440-66-6	metal
Acrolein	107-02-8	unknown
Aldrin	309-00-2	unknown
Benz[a]anthracene	56-55-3	unknown
Benzene hexachloride	608-73-1	unknown
Benzidine	92-87-5	unknown
Benz(e)acephenanthrylene	205-99-2	unknown
Benzo[a]pyrene	50-32-8	unknown
Benzoic acid	65-85-0	unknown
γ-Hexachlorocyclohexane (Lindane)	58-89-9	unknown
Bis(chloromethyl)ether	542-88-1	unknown
Chlordane	57-74-9	unknown
6-Chloro-m-cresol	59-50-7	unknown
Chrysene	218-01-9	unknown
Sodium cyanide	143-33-9	unknown
DDT	50-29-3	unknown
Dibenz[a,h]anthracene	53-70-3	unknown
Dibromochloromethane	124-48-1	unknown
2,4-Dichlorophenol	120-83-2	unknown
Dieldrin	60-57-1	unknown

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<u>Substance</u>	<u>CAS RN</u>	<u>Relative Dielectric Permittivity</u>
Diethyl phthalate	84-66-2	unknown
2,4-Dinitrophenol	51-28-5	unknown
2,4-Dinitrotoluene	121-14-2	unknown
2,6-Dinitrotoluene	606-20-2	unknown
Dioxins (TCDD)	1746-01-6	unknown
Endrin	72-20-8	unknown
Fluoranthene	206-44-0	unknown
Heptachlor	76-44-8	unknown
Hexachlorobenzene	118-74-1	unknown
Hexachloroethane	67-72-1	unknown
Isophorone	78-59-1	unknown
N-Nitrosodiphenylamine	86-30-6	unknown
Pentachlorophenol	87-86-5	unknown
Toxaphene	8001-35-2	unknown
2,4,6-Trichlorophenol	88-06-2	unknown

Table 9. Ranking of the 108 selected substances by electrical resistivity at room temperature (20°C), unless noted otherwise. Substances with the lowest resistivity (highest conductivity) appear at the top of the list. Resistivity is useful in predicting electrical property changes in ground water, soils, etc. in case of a spill or other discharge of the substances.

<u>Substance</u>	<u>CAS RN</u>	<u>Resistivity</u>
Silver	7440-22-4	$1.6 \times 10^{-14}$
Copper	7440-50-8	$1.7 \times 10^{-14}$ @ 22°C
Beryllium	7440-41-7	$3.3 \times 10^{-14}$ @ 22°C
Zinc	7440-66-6	$6. \times 10^{-14}$ @ 22°C
Cadmium	7440-43-9	$7.3 \times 10^{-14}$
Nickel	7440-02-0	$7.8 \times 10^{-14}$
Chromium	7440-47-3	$1.3 \times 10^{-13}$ @ 22°C
Thallium	7440-28-0	$1.6 \times 10^{-13}$
Lead	7439-92-1	$2.065 \times 10^{-13}$
Arsenic	7440-38-2	$2.9 \times 10^{-13}$ @ 22°C
Mercury	7439-97-6	$9.576 \times 10^{-13}$
Carbon disulfide	75-15-0	0.0000027
Tetrachloroethene	127-18-4	0.00001801
Ethylene glycol	107-21-1	0.00862
Hydrogen cyanide	74-90-8	0.0222 @ 18°C
Methanol	67-56-1	0.023 @ 18°C
Acrolein	107-02-8	0.0645
Ammonia	7664-41-7	0.0769 @ -79°C
4-Methyl-2-pentanone	108-10-1	<0.19 @ 35°C
Water	7732-18-5	0.227
Dibutyl phthalate	84-74-2	0.238 @ 30°C
Aniline	62-53-3	0.417 @ 25°C
Quinoline	91-22-5	0.45 @ 25°C
Acetone	67-64-1	0.5 @ 18°C
Bromoform	75-25-2	>0.5 @ 25°C
1,1-Dichloroethane	75-34-3	>0.5882 @ 25°C
Phenol	108-95-2	<0.59 @ 25°C
Trichloroethene	79-01-6	1.25
1,1,1-Trichloroethane	71-55-6	1.37
Acetic acid	64-19-7	1.67 @ 25°C
2-Butanone	78-93-3	2.78
Benzoic acid	65-85-0	3.3 @ 125°C
Chloroethane	75-00-3	>3.33 @ 0°C
Dimethyl sulfoxide	67-68-5	5. @ 25°C
Ethanol	64-17-5	7.41 @ 25°C
o-Cresol	95-48-7	7.69
Naphthalene	91-20-3	23.0 @ 81.8°C
1,2-Dichloroethane	107-06-2	33.3 @ 25°C
Nitrobenzene	98-95-3	48.8 @ 25°C
1,2-Dibromoethane	106-93-4	>50. @ 19°C
Chloroform	67-66-3	>100. @ 25°C
Chlorobenzene	108-90-7	143. @ 25°C
Dichloromethane	75-09-2	232.6 @ 25°C
1,2-dichlorobenzene	95-50-1	333. @ 25°C
Benzene	71-43-2	1316.

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<u>Substance</u>	<u>CAS RN</u>	<u>Resistivity</u>
1,4-Dioxane	123-91-1	$2. \times 10^6$ @ 25°C
<i>m</i> -Xylene	108-38-3	$1.16 \times 10^7$
<i>p</i> -Xylene	106-42-3	$1.3 \times 10^7$
<i>o</i> -Xylene	95-47-6	$1.5 \times 10^7$
Cyclohexane	110-82-7	$1.43 \times 10^9$ @ 25°C
Carbon tetrachloride	56-23-5	$2.5 \times 10^9$ @ 18°C
Toluene	108-88-3	$>1. \times 10^{10}$
Acrylonitrile	107-13-1	unknown
Aldrin	309-00-2	unknown
Aroclor 1260 (PCB 1260)	11096-82-5	unknown
Benz[ <i>a</i> ]anthracene	56-55-3	unknown
Benzene hexachloride	608-73-1	unknown
Benzidine	92-87-5	unknown
Benz( <i>e</i> )acephenanthrylene	205-99-2	unknown
Benzo[ <i>a</i> ]pyrene	50-32-8	unknown
<i>Bis</i> (2-chloroethyl)ether	111-44-4	unknown
<i>Bis</i> (chloromethyl)ether	542-88-1	unknown
<i>Bis</i> (2-ethylhexyl)phthalate	11-78-17	unknown
Bromomethane	74-83-9	unknown
Chlordane	57-74-9	unknown
6-Chloro- <i>m</i> -cresol	59-50-7	unknown
Chloromethane	74-87-3	unknown
Chrysene	218-01-9	unknown
DDT	50-29-3	unknown
Dibenz[ <i>a,h</i> ]anthracene	53-70-3	unknown
Dibromochloromethane	124-48-1	unknown
1,3-dichlorobenzene	541-73-1	unknown
1,4-dichlorobenzene	106-46-7	unknown
Dichlorodifluoromethane	75-71-8	unknown
1,1-Dichloroethene	75-35-4	unknown
<i>trans</i> -1,2-Dichloroethene	156-60-6	unknown
2,4-Dichlorophenol	120-83-2	unknown
1,2-Dichloropropane	78-87-5	unknown
Dieldrin	60-57-1	unknown
Diethyl phthalate	84-66-2	unknown
Dimethyl phthalate	131-11-3	unknown
2,4-Dinitrophenol	51-28-5	unknown
2,4-Dinitrotoluene	121-14-2	unknown
2,6-Dinitrotoluene	606-20-2	unknown
Dioxins (TCDD)	1746-01-6	unknown
Endrin	72-20-8	unknown
Ethylbenzene	100-41-4	unknown
Ethylene oxide	75-21-8	unknown
Fluoranthene	206-44-0	unknown
Heptachlor	76-44-8	unknown
Hexachlorobenzene	118-74-1	unknown
Hexachlorobutadiene	87-68-3	unknown
Hexachloroethane	67-72-1	unknown
$\gamma$ -Hexachlorocyclohexane (Lindane)	58-89-9	unknown
Isophorone	78-59-1	unknown
N-Nitrosodiphenylamine	86-30-6	unknown
Pentachlorophenol	87-86-5	unknown

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<u>Substance</u>	<u>CAS RN</u>	<u>Resistivity</u>
Phenanthrene	85-01-8	unknown
Potassium cyanide	151-50-8	unknown
Selenium	7782-49-2	unknown
Sodium cyanide	143-33-9	unknown
1,1,2,2-Tetrachloroethane	79-34-5	unknown
Toxaphene	8001-35-2	unknown
1,2,4-Trichlorobenzene	120-82-1	unknown
1,1,2-Trichloroethane	79-00-5	unknown
Trichlorofluoromethane	75-69-4	unknown
2,4,6-Trichlorophenol	88-06-2	unknown
Vinyl chloride	75-01-4	unknown
2,4-Xylenol	105-67-9	unknown

## 54 - Table 10

Table 10. The 108 selected substances ranked by ionization potential (in electron volts, eV). The ionization potential is used by various instruments to test atmospheres for the presence of toxic substances. Experimental methods for determining ionization potential are given in parentheses. The Chemical Abstracts Service Registry Numbers (CAS RN) are noted also.

EI = electron impact  
 PE = photoelectron spectroscopy  
 PI = photoionization  
 S = optical spectroscopy  
 VUS = vacuum ultraviolet spectroscopy

<u>Substance</u>	<u>CAS RN</u>	<u>Ionization Potential</u>	
		<u>eV</u>	<u>method</u>
Hydrogen cyanide	74-90-8	13.8	(EI)
Dichlorodifluoromethane	75-71-8	12.31	(PI)
Water	7732-18-5	12.6	(PI)
Trichlorofluoromethane	75-69-4	11.77	(PI)
Carbon tetrachloride	56-23-5	11.47	(PI)
Chloroform	67-66-3	11.42	(PI)
Dichloromethane	75-09-2	11.35	(PI)
Chloromethane	74-87-3	11.3	(PI,S)
1,2-Dichloroethane	107-06-2	11.12	(PI)
1,1-Dichloroethane	75-34-3	11.12	(PI)
1,1,2,2-Tetrachloroethane	79-34-5	11.10	(EI)
Chloroethane	75-00-3	10.97	(EI)
Acrylonitrile	107-13-1	10.91	(PI)
1,2-Dichloropropane	78-87-5	10.87	(PI)
Methanol	67-56-1	10.84	(PI,PE)
Dibromochloromethane	124-48-1	10.59	
Ethylene oxide	75-21-8	10.6	(PI,S)
Bromomethane	74-83-9	10.53	(S,PI)
Bromoform	75-25-2	10.51	(PI)
Ethanol	64-17-5	10.49	(PI)
Mercury	7439-97-6	10.43	(VUS)
Carbon disulfide	75-15-0	10.4	(S)
Acetic acid	64-19-7	10.36	(PI)
Ammonia	7664-41-7	10.2	(S,PI,PE)
1,2-Dibromoethane	106-93-4	10.19	(PI)
Acrolein	107-02-8	10.10	(PI)
Vinyl chloride	75-01-4	9.996	(S,PI)
Nitrobenzene	98-95-3	9.92	(PI)
Bis(2-chloroethyl)ether	111-44-4	9.85	
Arsenic	7440-38-2	9.81	(VUS)
Cyclohexane	110-82-7	9.8	(PI,PE)
Selenium	7782-49-2	9.75	(VUS)
Dimethyl phthalate	131-11-3	9.75	
Benzoic acid	65-85-0	9.73	(EI)
Acetone	67-64-1	9.69	(PI)
1,1-Dichloroethene	75-35-4	9.65	(PI)
<i>trans</i> -1,2-Dichloroethane	156-60-5	9.64	(PI)
2-Butanone	78-93-3	9.5	(PI)
Trichloroethene	79-01-6	9.45	(PI)

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Substance	CAS RN	Ionization Potential	
		eV	method
Zinc	7440-66-6	9.391	(S)
Beryllium	7440-41-7	9.32	(VUS)
Tetrachloroethene	127-18-4	9.32	(PI)
4-Methyl-2-pentanone	108-10-1	9.30	(PI)
Benzene	71-43-2	9.24	(S, PI)
1,4-Dioxane	123-91-1	9.13	(PI)
1,3-dichlorobenzene	541-73-1	9.12	(PI)
Chlorobenzene	108-90-7	9.07	(PI)
1,2-dichlorobenzene	95-50-1	9.06	(PI)
Cadmium	7440-43-9	8.991	(VUS)
o-Cresol	95-48-7	8.98	
1,4-dichlorobenzene	106-46-7	8.95	(PI)
Toluene	108-88-3	8.82	(PI)
Ethylbenzene	100-41-4	8.76	(PI)
m-Xylene	108-38-3	8.58	(PI, PE)
o-Xylene	95-47-6	8.56	(PI)
Fluoranthene	206-44-0	8.54	
Phenol	108-95-2	8.51	(PI)
p-Xylene	106-42-3	8.44	(PI)
Naphthalene	91-20-3	8.12	(PI)
Phenanthrene	85-01-8	8.1	(EI)
Benz[a]anthracene	56-55-3	8.01	(EI)
Chrysene	218-01-9	7.85	
Copper	7440-50-8	7.724	(VUS)
Aniline	62-53-3	7.7	(PI)
Nickel	7440-02-0	7.633	(VUS)
Silver	7440-22-4	7.574	(VUS)
Lead	7439-92-1	7.415	(VUS)
Dibenz[a,h]anthracene	53-70-3	7.28	
Chromium	7440-47-3	6.764	(VUS)
Thallium	7440-28-0	6.106	(VUS)
Aldrin	309-00-2	unknown	
Aroclor 1260 (PCB 1260)	11096-82-5	unknown	
Benzidine	92-87-5	unknown	
Benz(e)acephenanthrylene	205-99-2	unknown	
Benzo[a]pyrene	50-32-8	unknown	
Bis(chloromethyl)ether	542-88-1	unknown	
Bis(2-ethylhexyl)phthalate	117-81-7	unknown	
Chlordane	57-74-9	unknown	
6-Chloro-m-cresol	59-50-7	unknown	
DDT	50-29-3	unknown	
Dibutyl phthalate	84-74-2	unknown	
2,4-Dichlorophenol	120-83-2	unknown	
Dieldrin	60-57-1	unknown	
Diethyl phthalate	84-66-2	unknown	
Dimethyl sulfoxide	67-68-5	unknown	
2,4-Dinitrophenol	51-28-5	unknown	
2,4-Dinitrotoluene	121-14-2	unknown	
2,6-Dinitrotoluene	606-20-2	unknown	
Dioxins (TCDD)	1746-01-6	unknown	
Endrin	72-20-8	unknown	

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<u>Substance</u>	<u>CAS RN</u>	<u>Ionization Potential</u>	
		<u>eV</u>	<u>method</u>
Ethylene glycol	107-21-1	unknown	
Heptachlor	76-44-8	unknown	
Hexachlorobenzene	118-74-1	unknown	
Hexachlorobutadiene	87-68-3	unknown	
$\gamma$ -Hexachlorocyclohexane (Lindane)	58-89-9	unknown	
Hexachloroethane	67-72-1	unknown	
Isophorone	78-59-1	unknown	
N-Nitrosodiphenylamine	86-30-6	unknown	
Pentachlorophenol	87-86-5	unknown	
Potassium cyanide	151-50-8	unknown	
Quinoline	91-22-5	unknown	
Sodium cyanide	143-33-9	unknown	
Toxaphene	8001-35-2	unknown	
1,2,4-Trichlorobenzene	120-82-1	unknown	
1,1,1-Trichloroethane	71-55-6	unknown	
1,1,2-Trichloroethane	79-00-5	unknown	
2,4,6-Trichlorophenol	88-06-2	unknown	
2,4-Xylenol	105-67-9	unknown	



Table 11. Ranking of the 108 selected substances by fire hazard. The rating system is based primarily on flash points then explosive ranges in air. Substances at the top of the list are the most dangerous. At the bottom of the list are those substances for which nothing was found. Testing methods for lower and upper explosive limits in air (lel and uel) are noted if they were mentioned in the literature. The two methods most often used are the closed cup (CC) and open cup (OC). Some of the non-combustible substances may be ignited if they are in the form of dust or vapor, so were given a 'Low' rating rather than 'Very Low'. Ratings were determined as follows:

<u>Rating</u>	<u>flash point range</u>
Very high	$\leq 0^{\circ}\text{C}$
High	$0^{\circ}\text{C}-40^{\circ}\text{C}$ ( $32^{\circ}\text{F}-104^{\circ}\text{F}$ )
Moderate	$40^{\circ}\text{C}-100^{\circ}\text{C}$ ( $104^{\circ}\text{F}-212^{\circ}\text{F}$ )
Low	$>100^{\circ}\text{C}$
Very Low	non-combustible (NC)

<u>Substance</u>	<u>CAS RN</u>	<u>Flash point</u> <u><math>^{\circ}\text{C}</math></u>	<u>method</u>	<u>lel</u> <u>%</u>	<u>uel</u> <u>%</u>	<u>Rating</u>
Vinyl chloride	75-01-4	-78	(CC)	3.6	22	Very High
Chloroethane	75-00-3	-50	(CC)	3.8	15.4	Very High
Carbon disulfide	75-15-0	-30	(CC)	1.3	50	Very High
Acrolein	107-02-8	-25	(CC)	2.8	31	Very High
Ethylene oxide	75-21-8	-20	(OC)	3	100	Very High
Cyclohexane	110-82-7	-20	(CC)	1.33	8.35	Very High
Hydrogen cyanide	74-90-8	-18.8	(CC)	5.6	40	Very High
Acetone	67-64-1	-18	(CC)	2.6	12.8	Very High
1,1-Dichloroethene	75-35-4	-17.8	(OC)	7.3	16.0	Very High
Benzene	71-43-2	-11	(CC)	1.4	8.0	Very High
1,1-Dichloroethane	75-34-3	-5.6	(CC)	2.6	11.4	Very High
2-Butanone	78-93-3	-6.67	(CC)	1.8	11.5	Very High
Bis(chloromethyl)ether	542-88-1	-7.2	-	-	-	Very High
Acrylonitrile	107-13-1	-1.11	(CC)	3.1	17	Very High
Chloromethane	74-87-3	0	(CC)	8.1	17.2	Very High
<i>trans</i> -1,2-Dichloroethene	156-60-5	2.0	(CC)	9.7	12.8	High
Toluene	108-88-3	4	(CC)	1.0	7.3	High
Methanol	67-56-1	11	(CC)	6.0	36	High
1,4-Dioxane	123-91-1	12.2	(CC)	1.97	22.2	High
1,2-Dichloroethane	107-06-2	12.8	(CC)	6.2	15.9	High
Ethanol	64-17-5	13.11	(CC)	3.3	19	High
Ethylbenzene	100-41-4	15	(CC)	1.0	6.8	High
1,2-Dichloropropane	78-87-5	15.6	(CC)	3.4	14.5	High
4-Methyl-2-pentanone	108-10-1	16	(CC)	1.35	7.5	High
<i>o</i> -Xylene	95-47-6	17	(CC)	1.0	7	High
<i>p</i> -Xylene	106-42-3	27.2	(CC)	1.1	7.0	High
<i>m</i> -Xylene	108-38-3	28.9	(CC)	1.1	6.4	High
Chlorobenzene	108-90-7	29.4	(CC)	1.3	7.1	High
Trichloroethene	79-01-6	32	(CC)	8.0	10.5	High
Acetic acid	64-19-7	43	(CC)	5.4	16.0	Moderate
Bis(2-chloroethyl)ether	111-44-4	55	(CC)	-	-	Moderate
Chlordane	57-74-9	55.6	(CC)	-	-	Moderate
1,4-dichlorobenzene	106-46-7	65.5	-	-	-	Moderate

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<u>Substance</u>	<u>CAS RN</u>	<u>Flash point</u>		<u>lel</u>	<u>uel</u>	<u>Rating</u>
		°C	<u>method</u>	%	%	
1,2-dichlorobenzene	95-50-1	68.33	(CC)	2.2	9.2	Moderate
Aniline	62-53-3	70	(CC)	1.3	11	Moderate
DDT	50-29-3	72	(CC)	-	-	Moderate
Phenol	108-95-2	78	(CC)	1.7	8.6	Moderate
Naphthalene	91-20-3	78.9	(CC)	0.9	5.9	Moderate
o-Cresol	95-48-7	81.1		1.4	-	Moderate
Isophorone	78-59-1	84.4	(CC)	0.84	3.8	Moderate
Dimethyl sulfoxide	67-68-5	87.8	(CC)	2.6	28.5	Moderate
Nitrobenzene	98-95-3	87.8	(CC)	1.8	-	Moderate
1,2,4-Trichlorobenzene	120-82-1	98.9	(CC)	-	-	Moderate
Quinoline	91-22-5	107.2	(CC)	-	-	Low
2,4-Xylenol	105-67-9	>110		-	-	Low
Ethylene glycol	107-21-1	111.2	(CC)	3.2	-	Low
2,4-Dichlorophenol	120-83-2	113.8	(CC)	-	-	Low
Benzoic acid	65-85-0	121		-	-	Low
Toxaphene (liquid)	8001-35-2	135	(CC)	1.1	6.4	Low
Dimethyl phthalate	131-11-3	146	(CC)	1.2	-	Low
1,3-Dichlorobenzene	541-73-1	151	(CC)	2.02	9.2	Low
Dibutyl phthalate	84-74-2	157	(CC)	0.5	2.5	Low
Diethyl phthalate	84-66-2	163	(OC)	-	-	Low
Aroclor 1260 (PCB 1260)	11096-82-5	195	(CC)	-	-	Low
2,4-Dinitrotoluene	121-14-2	206.7	(CC)	-	-	Low
Bis(2-ethylhexyl)phthalate	117-81-7	218	(OC)	-	-	Low
Hexachlorobenzene	118-74-1	242		-	-	Low
2,6-Dinitrotoluene	606-20-2	404	(CC)	-	-	Low
2,4-Dinitrophenol	51-28-5	???	(combustible)	-	-	Low
Phenanthrene	85-01-8	NC	?			Low
Ammonia	7664-41-7	NC				Low
Arsenic	7440-38-2	NC				Low
Beryllium	7440-41-7	NC	(comb. dust)			Low
Cadmium	7440-43-9	NC	(comb. dust)			Low
Chromium	7440-47-3	NC	(comb. dust)			Low
Copper	7440-50-8	NC	(comb. dust)			Low
Lead	7439-92-1	NC	(comb. dust)			Low
Nickel	7440-02-0	NC	(comb. dust)			Low
Silver	7440-22-4	NC	(comb. dust)			Low
Thallium	7440-28-0	NC	(comb. dust)			Low
Zinc	7440-66-6	NC	(comb. dust)			Low
Hexachloroethane	67-72-1	NC				Very Low
1,1,1-Trichloroethane	71-55-6	NC				Very Low
1,1,2,2-Tetrachloroethane	79-34-5	NC				Very Low
1,1,2-Trichloroethane	79-00-5	NC				Very Low
2,4,6-Trichlorophenol	88-06-2	NC				Very Low
Aldrin	309-00-2	NC				Very Low
Benzene hexachloride	608-73-1	NC				Very Low
Benzidine	92-87-5	NC				Very Low
Bromoform	75-25-2	NC				Very Low
Bromomethane	74-83-9	NC				Very Low
Carbon tetrachloride	56-23-5	NC				Very Low
Chloroform	67-66-3	NC				Very Low
Dibromochloromethane	124-48-1	NC				Very Low

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<u>Substance</u>	<u>CAS RN</u>	<u>Flash point</u>		<u>lel</u>	<u>uel</u>	<u>Rating</u>
		°C	<u>method</u>	%	%	
1,2-Dibromoethane	106-93-4	NC				Very Low
Dichlorodifluoromethane	75-71-8	NC				Very Low
Dichloromethane	75-09-2	NC				Very Low
Dieldrin	60-57-1	NC				Very Low
Endrin	72-20-8	NC				Very Low
Heptachlor	76-44-8	NC				Very Low
Hexachlorobutadiene	87-68-3	NC				Very Low
γ-Hexechlorocyclohexane	58-89-9	NC				Very Low
Mercury	7439-97-6	NC				Very Low
N-Nitrosodiphenylamine	86-30-6	NC				Very Low
Pentachlorophenol	87-86-5	NC				Very Low
Potassium cyanidem	151-50-8	NC				Very Low
Selenium	7782-49-2	NC				Very Low
Sodium cyanide	143-33-9	NC				Very Low
Tetrachloroethene	127-18-4	NC				Very Low
Trichlorofluoromethane	75-69-4	NC				Very Low
Water	7732-18-5	NC				Very Low
6-Chloro-m-cresol	59-50-7	Unknown				
Benz[a]anthracene	56-55-3	Unknown				
Benz(e)acephenanthrylene	205-99-2	Unknown				
Benzo[a]pyrene	50-32-8	Unknown				
Chrysene	218-01-9	Unknown				
Dibenz[a,h]anthracene	53-70-3	Unknown				
Fluoranthene	206-44-0	Unknown				
Dioxins (TCDD)	1746-01-6	Unknown				

## 60 - Table 12

Table 12. References for clay-organic interactions for the 108 selected substances. For general reference, see Goring and Hamaker (1972), Theng (1974), MacEwan and Wilson (1980), Rausell-Colom and Serratosa (1987), or Dragun (1988). Unknown means nothing was found. Inorganics typically involve cation exchange, but are otherwise not discussed further.

<u>Substance</u>	<u>CAS RN</u>	<u>Interaction Reference</u>
Acetic Acid	64-19-7	Brindley and Moll, 1965 Carr and Chih, 1971 Larson and Sherman, 1964 Lord et al., 1983
Acetone	67-64-1	Acar et al., 1984, 1985 Anderson and Brown, 1981 Barshad, 1952 Bissada et al., 1967 Brindley et al., 1969 Brown and Thomas, 1984 Brown et al., 1983, 1984, 1986 Carr and Chih, 1971 Griffin et al., 1984 Glaeser, 1948 Lord et al., 1983 Mortland, 1970 Ruiz-Amil and MacEwan, 1957
Acrolein	107-02-8	Theng, 1974
Acrylonitrile	107-13-1	Blumstein et al., 1974 Greenland, 1972 Mortensen, 1959 Mortensen, 1962 Yamanaka et al., 1971
Aldrin	309-00-2	Kenega and Goring, 1980
Ammonia	7664-41-7	Mortland et al., 1963 Russell, 1965
Aniline	62-53-3	Anderson and Brown, 1981 Anderson et al., 1981 Briggs, 1981 Brown et al., 1984 Evans et al., 1985 Greene-Kelly, 1955 Furukawa and Brindley, 1973 Heller and Yariv, 1969 Pillai et al., 1982 Tennakoon et al., 1974 Yariv et al., 1968, 1969
Arsenic	7440-38-2	inorganic
Aroclor 1260 (PCB 1260)	11096-82-5	Dragun and Helling, 1985
Benz[a]anthracene	56-55-3	unknown

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<u>Substance</u>	<u>CAS RN</u>	<u>Interaction Reference</u>
Benzene	71-43-2	Acar et al., 1984, 1985 Barshad, 1952 Chiou et al., 1983 Doner and Mortland, 1969 Greene-Kelly, 1955 Karickhoff et al., 1979 Pinnavaia and Mortland, 1971 Rodgers et al., 1980 Serratosa, 1968 Vandepoel et al., 1973
Benzidine	92-87-5	Furukawa and Bridley, 1973 Greene-Kelly, 1955 McBride, 1985
Benz(e)acephenanthrylene	205-99-2	unknown
Benzo[a]pyrene	50-32-8	unknown
Benzoic acid	65-85-0	Greene-Kelly, 1955 Yariv et al., 1966
Beryllium	7440-41-7	inorganic
Bis(2-chloroethyl)ether	111-44-4	unknown
Bis(chloromethyl)ether	542-88-1	unknown
Bis(2-ethylhexyl)phthalate	117-81-7	unknown
Bromoform	75-25-2	unknown
Bromomethane	74-83-9	unknown
2-Butanone	78-93-3	unknown
Cadmium	7440-43-9	inorganic
Carbon disulfide	75-15-0	inorganic
Carbon tetrachloride	56-23-5	Evans et al., 1985 Rogers and McFarlane, 1981
Chlordane	57-74-9	unknown
Chlorobenzene	108-90-7	Chiou et al., 1983 Greene-Kelly, 1955 Serratosa, 1968
6-Chloro-m-cresol	59-50-7	unknown
Chloroethane	75-00-3	unknown
Chloroform	67-66-3	unknown
Chloromethane	74-87-3	unknown
Chromium	7440-47-3	inorganic
Chrysene	218-01-9	unknown
Copper	7440-50-8	inorganic
o-Cresol	95-48-7	Erickson, 1948 Greene-Kelly, 1955
Cyclohexane	110-82-7	Rao et al., 1988
DDT	50-29-3	Fleck and Haller, 1945 Huang and Liao, 1970 Karickhoff, 1981 Kenega and Goring, 1980 McCall et al., 1980 Richardson and Epstein, 1971
Dibenz[a,h]anthracene	53-70-3	unknown
Dibromochloromethane	124-48-1	unknown
1,2-Dibromoethane	106-93-4	Rogers and McFarlane, 1981
Dibutyl phthalate	84-74-2	unknown

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<u>Substance</u>	<u>CAS RN</u>	<u>Interaction Reference</u>
1,2-dichlorobenzene	95-50-1	Chiou et al., 1983
1,3-dichlorobenzene	541-73-1	Chiou et al., 1983
1,4-dichlorobenzene	106-46-7	Chiou et al., 1983
Dichlorodifluoromethane	75-71-8	unknown
1,1-Dichloroethane	75-34-3	unknown
1,2-Dichloroethane	107-06-2	Karickhoff, 1981
		Rao et al., 1988
1,1-Dichloroethene	75-35-4	unknown
<i>trans</i> -1,2-Dichloroethene	156-60-5	Rao et al., 1988
Dichloromethane	75-09-2	unknown
2,4-Dichlorophenol	120-83-2	Davidson et al., 1980
		Artiola-Fortung and Fuller, 1982
1,2-Dichloropropane	78-87-5	unknown
Dieldrin	60-57-1	Boucher and Lee, 1972
		Fowker et al., 1960
		Huang and Liao, 1970
Diethyl phthalate	84-66-2	unknown
Dimethyl phthalate	131-11-3	unknown
Dimethyl sulfoxide	67-68-5	Andrews et al., 1967
		Jacobs and Sterckx, 1970
2,4-Dinitrophenol	51-28-5	unknown
2,4-Dinitrotoluene	121-14-2	unknown
2,6-Dinitrotoluene	606-20-2	unknown
1,4-Dioxane	123-91-1	Brindley et al., 1969
		Brindley and Tsunashima, 1972
		Carr and Chih, 1971
		Griffin et al., 1984
		Hoffmann and Brindley, 1962
		Greenland et al., 1965a, 1965b
Dioxins (TCDD)	1746-01-6	unknown
Endrin	72-20-8	Fowker et al., 1960
Ethanol	64-17-5	Barshad, 1952
		Bissada, 1967
		Brindley et al., 1969
		Dandy and Nadiye-Tabbiruk, 1982
		Dowdy and Mortland, 1967
		Griffin et al., 1984
		Mesri and Olson, 1971
		Mortland, 1970
		Stul, 1985
Ethylbenzene	100-41-4	Chiou et al., 1983
		Rao et al., 1988
Ethylene oxide	75-21-8	unknown

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<u>Substance</u>	<u>CAS RN</u>	<u>Interaction Reference</u>
Ethylene glycol	107-21-1	Anderson and Brown, 1981 Anderson and Jones, 1983 Brindley, 1966 Dowdy and Mortland, 1968 Greenland, 1972 Griffin et al., 1984 Hoffmann and Brindley, 1961 Lord et al., 1983 Mortland, 1970 Parfitt and Greenland, 1970 Reynolds, 1965 Schramm et al., 1986 Walker, 1958
Fluoranthene	206-44-0	unknown
Heptachlor	76-44-8	Huang and Liao, 1970 Malina et al., 1956
Hexachlorobenzene	118-74-1	Dragun and Helling, 1985
Hexachlorobutadiene	87-68-3	unknown
$\gamma$ -Hexachlorocyclohexane (Lindane)	58-89-9	Boucher and Lee, 1972 Karickhoff, 1981 Lotse et al., 1968 McCall et al., 1980
Hexachloroethane	67-72-1	unknown
Hydrogen cyanide	74-90-8	unknown
Isophorone	78-59-1	unknown
Lead	7439-92-1	inorganic
Mercury	7439-97-6	inorganic
Methanol	67-56-1	Anderson et al., 1981, 1985 Brindley et al., 1969 Foreman and Daniel, 1984 Griffin et al., 1984 Lord et al., 1983 Theng, 1974
4-Methyl-2-pentanone	108-10-1	unknown
Naphthalene	91-20-3	Karickhoff et al., 1979 MacEwan, 1948
Nickel	7440-02-0	inorganic
Nitrobenzene	98-95-3	Acar et al., 1984, 1985 Barshad, 1952 Briggs, 1981 Greene-Kelly, 1955 Yariv et al., 1966
N-Nitrosodiphenylamine	86-30-6	unknown
Pentachlorophenol	87-86-5	Choi and Aomine, 1974 Kenega and Goring, 1980 Nose, 1966
Phenanthrene	85-01-8	Karickhoff et al., 1979

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<u>Substance</u>	<u>CAS RN</u>	<u>Interaction Reference</u>
Phenol	108-95-2	Acar et al., 1985 Artiola-Fortung and Fuller, 1982 Erickson, 1948 Fenn and Mortland, 1973 Greene-Kelly, 1955 Isaacson and Sawhney, 1983 Kenega and Goring, 1980 Wang et al., 1978
Potassium cyanide	151-50-8	unknown
Quinoline	91-22-5	Doehler and Young, 1962 Greene-Kelly, 1955 Helmy et al., 1983 Kutilek and Slangerova, 1966 Yamamoto et al., 1969
Selenium	7782-49-2	inorganic
Silver	7440-22-4	inorganic
Sodium cyanide	143-33-9	unknown
1,1,2,2-Tetrachloroethane	79-34-5	Karickhoff, 1981 Rao et al., 1988
Tetrachloroethene	127-18-4	Karickhoff, 1981
Thallium	7440-28-0	inorganic
Toluene	108-88-3	Doner and Mortland, 1969 Pinnavaia and Mortland, 1971 Pinnavaia et al., 1974 Rao et al., 1988 Sadowski, 1988
Toxaphene	8001-35-2	LaFleur, 1974
1,2,4-Trichlorobenzene	120-82-1	Chiou et al., 1983
1,1,1-Trichloroethane	71-55-6	Karickhoff, 1981
1,1,2-Trichloroethane	79-00-5	unknown
Trichloroethene	79-01-6	Anderson et al., 1985 Brown and Thomas, 1984 Rao et al., 1988 Rogers and McFarlane, 1981
Trichlorofluoromethane	75-69-4	unknown
2,4,6-Trichlorophenol	88-06-2	Rosenfield and van Valkenburg, 1965
Vinyl chloride	75-01-4	unknown
Water	7732-18-5	Elprince, 1986 Greenland and Hayes, 1981 Newman, 1987 Sposito, 1984 van Olphen, 1977 Yariv and Cross, 1979



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<u>Substance</u>	<u>CAS RN</u>	<u>Interaction Reference</u>
m-Xylene	108-38-3	See p-Xylene
o-Xylene	95-47-6	See p-Xylene
p-Xylene	106-42-3	Anderson and Brown, 1981
		Anderson and Jones, 1983
		Anderson et al., 1981
		Brown and Thomas, 1984
		Brown et al., 1986
		Lord et al., 1983
		Pinnavaia and Mortland, 1971
		Rao et al., 1988
		Schramm et al., 1986
2,4-Xylenol	105-67-9	unknown
Zinc	7440-66-6	inorganic

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Table 13. Threshold Limit Values (TLVs) for the 108 selected hazardous substances. Values are taken from the American Conference of Governmental Industrial Hygienists publication "Threshold Limit Values and Biological Exposure Indices for 1988-1989". Refer to the definition section of this report and the above booklet for more complete discussions of TLVs.

- A1 Confirmed human carcinogen
- A2 Suspected human carcinogen
- C Ceiling limit
- STEL Short-term Exposure Limit
- TWA Time-Weighted 8-hour Average
- ◆ Substance for which OSHA or NIOSH has a Permissible Exposure Limit (PEL) or a Recommended Exposure Limit (REL) less than the TLV
- Substance identified by other sources as a suspected or confirmed human carcinogen.

<u>TWA</u>		<u>STEL</u>		<u>Substance</u>	<u>CAS RN</u>
ppm	(mg/m <sup>3</sup> )	ppm	(mg/m <sup>3</sup> )		
10	25	15	(37)	Acetic acid	64-19-7
750	1780	1000	(2375)	◆Acetone	67-64-1
0.1	(0.25)	0.	(0.8)	Acrolein	107-02-8
2, A2	4.5), A2	-	- (skin)	◆■Acrylonitrile	107-13-1
-	0.25)	-	- (skin)	Aldrin	309-00-2
25	18	35	(27)	Ammonia	7664-41-7
2	10	-	- (skin)	■Aniline	62-53-3
-	0.2	-	-	◆■Arsenic	7440-38-2
-	0.2 , A2	-	-	Benz[a]anthracene(coal tar)	56-55-3
10, A2	30, A2	-	-	◆■Benzene	71-43-2
-	A1	-	- (skin)	■Benzidine	92-87-5
-	-	-	-	Benz(e)acephenanthrylene	205-99-2
-	A2	-	-	■Benzo[a]pyrene	50-32-8
-	-	-	-	Benzoic acid	65-85-0
-	0.002, A2	-	-	◆■Beryllium	7440-41-7
5	30	10	60	Bis(2-chloroethyl)ether	111-44-4
-	5	-	10	◆■Bis(2-ethylhexyl)phthalate	117-81-7
0.001	0.005	-	-	◆■Bis(chloromethyl)ether	542-88-1
0.5	5	-	- (skin)	Bromoform	75-25-2
5	20	-	- (skin)	Bromomethane	74-83-9
200	590	300	885	2-Butanone	78-93-3
-	0.05	-	-	Cadmium	7440-43-9
10	30	-	- (skin)	◆Carbon disulfide	75-15-0
5, A2	30, A2	-	- (skin)	◆■Carbon tetrachloride	56-23-5
-	0.5	-	2 (skin)	■Chlordane	57-74-9
75	350	-	-	Chlorobenzene	108-90-7
-	-	-	-	6-Chloro-m-cresol	59-50-7
1000	2600	-	-	Chloroethane	75-00-3
10, A2	50, A2	-	-	Chloroform	67-66-3
50	105	100	205	◆■Chloromethane	74-87-3
-	0.05	-	-	Chromium (metal)	7440-47-3
A2	A2	-	-	■Chrysene	218-01-9
-	0.2	-	-	Copper (fume, dust, mist)	7440-50-8

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<u>TWA</u>		<u>STEL</u>			<u>Substance</u>	<u>CAS RN</u>
ppm	(mg/m <sup>3</sup> )	ppm	(mg/m <sup>3</sup> )			
5	22	-	-	(skin)	<i>o</i> -Cresol	95-48-7
300	1050	-	-		Cyclohexane	110-82-7
-	1	-	-		◆DDT	50-29-3
-	-	-	-		Dibenz[ <i>a,h</i> ]anthracene	53-70-3
-	-	-	-		Dibromochloromethane	124-48-1
A2	A2	-	-		◆1,2-Dibromoethane	106-93-4
-	5	-	-		Dibutyl phthalate	84-74-2
-	-	-	-		1,3-dichlorobenzene	541-73-1
C 50	C 300	-	-		1,2-dichlorobenzene	95-50-1
75	450	110	675		1,4-dichlorobenzene	106-46-7
1000	4950	-	-		Dichlorodifluoromethane	75-71-8
200	810	250	1010		◆1,1-Dichloroethane	75-34-3
10	40	-	-		◆1,2-Dichloroethane	107-06-2
5	20	20	80		◆1,1-Dichloroethene	75-35-4
-	-	-	-		<i>trans</i> -1,2-Dichloroethene	156-60-5
50,A2	175,A2	-	-		◆Dichloromethane	75-09-2
-	-	-	-		2,4-Dichlorophenol	120-83-2
75	350	110	510		1,2-Dichloropropane	78-87-5
-	0.25	-	-	(skin)	◆Dieldrin	60-57-1
-	5	-	-		Diethyl phthalate	84-66-2
-	5	-	-		Dimethyl phthalate	131-11-3
-	-	-	-		Dimethyl sulfoxide	67-68-5
-	-	-	-		2,4-Dinitrophenol	51-28-5
-	1.5	-	-	(skin)	◆2,4-Dinitrotoluene	121-14-2
-	-	-	-		2,6-Dinitrotoluene	606-20-2
25	90	-	-	(skin)	◆1,4-Dioxane	123-91-1
-	-	-	-		Dioxins (TCDD)	1746-01-6
-	0.1	-	-	(skin)	Endrin	72-20-8
1000	1900	-	-		Ethanol	64-17-5
100	435	125	545		Ethylbenzene	100-41-4
C 50	C 450	-	-		Ethylene glycol	107-21-1
1,A2	2,A2	-	-		■Ethylene oxide	75-21-8
-	-	-	-		Fluoranthene	206-44-0
-	0.5	-	-	(skin)	Heptachlor	76-44-8
-	-	-	-		Hexachlorobenzene	118-74-1
0.02	0.24,A2	-	-	(skin)	Hexachlorobutadiene	87-68-3
-	0.5	-	-	(skin)	■γ-Hexachlorocyclohexane	58-89-9
1	10	-	-		Hexachloroethane	67-72-1
-	5	-	-	(skin)	Hydrogen	74-90-8
C 5	C 25	-	-		Isophorone	78-59-1
-	0.15	-	-		Lead (dusts, fumes)	7439-92-1
-	0.01	-	0.03		Mercury (alkyl cmpds)	7439-97-6
-	0.05	-	-		Mercury	
-	0.1	-	-		(all exc. alkyl cmpds.)	7439-97-6
					◆Mercury	
					(aryl and inorg. cmpds)	7439-97-6
200	260	250	310		Methanol	67-56-1
50	205	75	300		4-Methyl-2-pentanone	108-10-1
10	50	15	75		Naphthalene	91-20-3
-	1	-	-		■Nickel (metal)	7440-02-0
1	5	-	-	(skin)	Nitrobenzene	98-95-3

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<u>TWA</u>		<u>STEL</u>		<u>Substance</u>	<u>CAS RN</u>
ppm	(mg/m <sup>3</sup> )	ppm	(mg/m <sup>3</sup> )		
-	-	-	-	N-Nitrosodiphenylamine	86-30-6
-	1	-	2	(skin) PCB (42% Cl)	53469-21-9
-	0.5	-	1	(skin) PCB (54% Cl)	11097-69-1
-	0.5	-	-	(skin) Pentachlorophenol	87-86-5
-	-	-	-	Phenanthrene	85-01-8
5	19	-	-	(skin) Phenol	108-95-2
-	5	-	-	(skin) Potassium cyanide	151-50-8
-	-	-	-	Quinoline	91-22-5
-	0.2	-	-	Selenium	7782-49-2
-	0.1	-	-	Silver (metal)	7440-22-4
-	0.01	-	-	Silver (soluble cmpds.)	7440-22-4
-	5	-	-	(skin) Sodium cyanide	143-33-9
1	7	-	-	(skin) ◆■1,1,2,2-Tetrachloroethane	79-34-5
50	335	200	1340	◆Tetrachloroethene	127-18-4
-	0.1	-	-	(skin) Thallium (soluble cmpds.)	7440-28-0
100	375	150	560	Toluene	108-88-3
-	0.5	-	1	(skin) Toxaphene	8001-35-2
C 5	C 40	-	-	1,2,4-Trichlorobenzene	120-82-1
350	1900	450	2450	◆1,1,1-Trichloroethane	71-55-6
10	45	-	-	(skin) ◆■1,1,2-Trichloroethane	79-00-5
50	270	200	1080	◆■Trichloroethene	79-01-6
C 1000	C 5600	-	-	Trichlorofluoromethane	75-69-4
-	-	-	-	2,4,6-Trichlorophenol	88-06-2
5,A2	10,A2	-	-	◆■Vinyl chloride	75-01-4
-	-	-	-	Water	7732-18-5
100	435	150	665	m-Xylene	108-38-3
100	435	150	665	o-Xylene	95-47-6
100	435	150	665	p-Xylene	106-42-3
-	-	-	-	2,4-Xylenol	105-67-9
-	-	-	-	Zinc (metal)	7440-66-6

Table 14. Maximum Contaminant Level Goals (MCLGs) and Maximum Contaminant Levels (MCLs) for drinking water contaminants in the U.S. The standards were or will be established by the U.S. Environmental Protection Agency (EPA) as required by the Safe Drinking Water Act (SDWA) Amendments of 1986. All current drinking water regulations may be found in the Code of Federal Regulations (CFR) Volume 40, Parts 141, 142, and 143. Regulations published between CFR regulations may be found in the Federal Register. The MCLG is a level to be established at which no known or anticipated adverse effects on the health of persons occur and which allows an adequate safety margin. By policy, the EPA sets MCLGs at zero for known or probable human carcinogens. The MCL is the maximum permissible level of a contaminant in water which is deliverable to any user of a public water system. The MCL is to be established as close to the MCLG as feasible. The MCLG is a non-enforceable health-based goal and the MCL is an enforceable standard that public water systems must meet. There are two types of drinking water standards: primary MCLs and secondary MCLs. Primary MCLs are set for substances that are of a concern for health and are enforceable. Secondary MCLs serve as guidelines in setting levels based on aesthetic considerations such as taste or odor and are not federally enforceable. Contaminants with asterisks are included in this report. Values are in milligram/liter (mg/l) unless noted otherwise. Other abbreviations are mrem/yr (millirem per year) and pCi/l (picoCurie per liter).

■ Final Rule

§ Proposed August 18, 1988; Final rule expected Spring 1990

T Proposed May 27, 1989; Final rule expected December 1990

† To be proposed March 1990 (as of June 1989); Final rule expected Spring 1991

♦ To be proposed June 1990 (as of June 1989); Final rule expected Summer 1991

	<u>MCLG (mg/l)</u>	<u>MCL (mg/l)</u>
<u>Volatile Organic Chemicals</u>		
*Benzene	■ zero	■ 0.005
*Carbon Tetrachloride	■ zero	■ 0.005
*Chlorobenzene	T 0.1	T 0.1
*Dichlorobenzene(s) (1,4 isomer)	■ 0.075	■ 0.075
(1,2 isomer)	T 0.6	T 0.6
*1,2-Dichloroethane	■ zero	■ 0.005
*1,1-Dichloroethene	■ 0.007	■ 0.007
*cis-1,2-Dichloroethene	T 0.07	T 0.07
*trans-1,2-Dichloroethene	T 0.1	T 0.1
*Dichloromethane (Methylene Chloride)	† zero	
*Tetrachloroethene	T zero	T 0.005
*1,1,1-Trichloroethane	■ 0.2	■ 0.2
*Trichloroethene (TCE)	■ zero	■ 0.005
*Trichlorobenzene(s) (1,2,4 isomer)	† 0.009	
*Vinyl Chloride	■ zero	■ 0.002

	<u>MCLG (mg/l)</u>	<u>MCL (mg/l)</u>
<u>Synthetic Organic Chemicals/Pesticides</u>		
Adipates (di(ethylhexyl) adipate)	† 0.5	
Alachlor	T zero	T 0.002
Aldicarb	T 0.01	T 0.01
Aldicarb Sulfoxide	T 0.01	T 0.01
Aldicarb Sulfone	T 0.04	T 0.04
Atrazine	T 0.003	T 0.003
Carbofuran	T 0.04	T 0.04
*Chlordane	T zero	T 0.002
2,4-D	T 0.07	T 0.07
Dalapon	† 0.07	
Dibromochloropropane (DBCP)	T zero	T 0.0002
*1,2-Dichloropropane	T zero	T 0.005
Dinoseb	† 0.007	
Diquat	† 0.02	
Endothall	† 0.1	
*Endrin	† 0.002	
*Ethylbenzene	T 0.7	T 0.7
Ethylene Dibromide (EDB)	T zero	T 0.00005
Glyphosate	† 0.7	
*Heptachlor	T zero	T 0.0004
Heptachlor Epoxide	T zero	T 0.0002
*Hexachlorobenzene	† zero	
Hexachlorocyclopentadiene	† 0.05	
*Lindane	T 0.0002	T 0.0002
Methoxychlor	T 0.4	T 0.4
Oxamyl (Vydate)	† 0.2	
*PAHs (Polynuclear Aromatic Hydrocarbons)		
(Benzo(a)pyrene)	† zero	
*Polychlorinated Biphenyls (PCBs)		
(as decachlorobiphenyl)	T zero	T 0.0005
*Pentachlorophenol	T 0.2	T 0.2
*Phthalates (Di(ethylhexyl) phthalate)	† zero	
Pichloram	† 0.5	
*2,3,7,8-TCDD (Dioxin)	† zero	
2,4,5-TP (Silvex)	T 0.05	T 0.05
Simazine	† 0.004	
Styrene		
(based on Group B <sub>2</sub> carcinogen classification)	T 0	T 0.005
(based on Group C carcinogen classification)	T 0.1	T 0.1
*Toluene	T 2	T 2
*Toxaphene	T zero	T 0.005
*1,1,2-Trichloroethane	† 0.003	
*Total Trihalomethanes (chloroform, bromoform bromodichloromethane)		0.1
*Xylene (total)	T 10	T 10

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	<u>MCLG (mg/l)</u>	<u>MCL (mg/l)</u>
<u>Inorganic Chemicals</u>		
Antimony	† 0.003	
*Arsenic	† 0	
Asbestos (longer than 10 µm)	T 7 million fibers/l (both)	
Barium	T 5	T 5
*Beryllium	† zero	
*Cadmium	T 0.005	T 0.005
*Chromium	T 0.1	T 0.1
*Copper (secondary standard)	§ 1.3	§ 1.3
*Cyanide	† 0.2	
Fluoride	■ 4.0	■ 4.0
*Lead	§ zero	§ 0.005
*Mercury	T 0.002	T 0.002
*Nickel	† 0.1	
Nitrate (as N)	T 10	T 10
Nitrite (as N)	T 1	T 1
Total Nitrate and Nitrite	T 10	T 10
*Selenium	T 0.05	T 0.05
Sulfate	† 200-400	
*Thallium	† 0.0004	
<u>Water Treatment Chemicals</u>		
Acrylamide	T zero	NA
Epichlorohydrin	T zero	NA
<u>Radiological Contaminants</u>		
Radium 226 and 228	♦ zero	♦ 5 pCi/l
Gross Alpha Particle Activity	♦ zero	♦ 15 pCi/l
Beta Particle and Photon Radioactivity	♦ zero	♦ 4 mrem/yr
Natural Uranium	♦ zero	♦ 20-40 pCi/l
Radon-222 (in water)	♦ zero	♦ 200-2000 pCi/l
<u>Microbial Contaminants</u>		
Total Coliform	■ zero	NA
<i>Giardia lamblia</i>	■ zero	NA
Heterotrophic Plate Count (HCP)	■ none	NA
<i>Legionella</i>	■ zero	NA
Turbidity	■ none	NA
Viruses	■ zero	NA

(Treatment technique requirements are established in lieu of MCLs for microbial contaminants and water treatment chemicals.)

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Table 15. Chemicals on the EPA top 100 hazardous substances list that are not included in this report because of insufficient data. The Chemical Abstracts Service Registry Number (CAS RN) and Priority Group (PG) are noted (see Table 1). PAH = polynuclear aromatic hydrocarbon.

<u>CAS RN</u>	<u>PG</u>	<u>Substance</u>
62-75-9	2	n-Nitrosodimethylamine
72-54-8	2	DDD (listed with DDT 50-29-3)
72-55-9	2	4,4'-DDE (listed with DDT 50-29-3)
75-27-4	2	Bromodichloromethane
91-94-1	2	3,3'-Dichlorobenzidine
122-66-7	3	1,2-Diphenylhydrazine
193-39-5	3	Indeno(1,2,3-cd)pyrene (refer to other PAHs)
319-84-6	2	alpha-BHC (listed with $\gamma$ -hexachlorocyclohexane 58-89-9)
319-85-7	2	beta-BHC (listed with $\gamma$ -hexachlorocyclohexane 58-89-9)
319-86-8	2	delta-BHC (listed with $\gamma$ -hexachlorocyclohexane 58-89-9)
621-64-7	2	n-Nitrosodi-n-propylamine
1024-57-3	1	Heptachlor epoxide (listed with heptachlor 76-44-8)
7221-93-4	3	Endrin aldehyde (listed with endrin 72-20-8)
-----	1	PCB-54,48,42,32,21,1016 (listed with PCB-1260 11196-82-5)



Table 16. Classification of the selected 107 substances by use (water is not included). Substances may appear in more than one classification and not all uses are given for a particular substance. The Chemical Abstracts Service Registry Number (CAS RN) is given for each substance.

<u>Substance</u>	<u>CAS RN</u>
<u>Chemical processing or manufacturing/plastics/organic synthesis</u>	
Acetic acid	64-19-7
Acrolein	107-02-8
Acrylonitrile	107-13-1
Ammonia	7664-41-7
Aniline	62-53-3
Benzene	71-43-2
Benzidine	92-87-5
Benzoic acid	65-85-0
Bis(chloromethyl) ether	542-88-1
Bis(2-ethylhexyl) phthalate	117-81-7
Carbon disulfide	75-15-0
Carbon tetrachloride	56-23-5
Chlorobenzene	108-90-7
Chloroethane	75-00-3
Chloromethane	74-87-3
Chromium	7440-47-3
o-Cresol	95-48-7
Cyclohexane	110-82-7
Dibromochloromethane	124-48-1
1,2-Dibromoethane	106-93-4
Dibutyl phthalate	84-74-2
1,2-Dichlorobenzene	95-50-1
Dichlorodifluoromethane	75-71-8
1,1-Dichloroethane	75-34-3
1,2-Dichloroethane	107-06-2
1,1-Dichloroethene	75-35-4
trans-1,2-Dichloroethene	156-60-5
Dichloromethane	75-09-2
2,4-Dichlorophenol	120-83-2
1,2-Dichloropropane	78-87-5
Diethyl phthalate	84-66-2
Dimethyl phthalate	131-11-3
Dimethyl sulfoxide	67-68-5
2,4-Dinitrophenol	51-28-5
2,4-Dinitrotoluene	121-14-2
2,6-Dinitrotoluene	606-20-2
1,4-Dioxane	123-91-1
Ethanol	64-17-5
Ethylbenzene	100-41-4
Ethylene glycol	107-21-1
Ethylene oxide	75-21-8
Hexachlorobenzene	118-74-1
Hexachlorobutadiene	87-68-3
Hexachloroethane	67-72-1
Hydrogen cyanide	74-90-8
Isophorone	78-59-1

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<u>Substance</u>	<u>CAS RN</u>
Methanol	67-56-1
4-Methyl-2-pentanone	108-10-1
Naphthalene	91-20-3
Nitrobenzene	98-95-3
Pentachlorophenol	87-86-5
Quinoline	91-22-5
Sodium cyanide	143-33-9
1,1,2,2-Tetrachloroethane	79-34-5
Tetrachloroethene	127-18-4
Thallium	7440-28-0
Toluene	108-88-3
1,1,2-Trichloroethane	79-00-5
Trichloroethene	79-01-6
Trichlorofluoromethane	75-69-4
2,4,6-Trichlorophenol	88-06-2
Vinyl chloride	75-01-4
<i>m</i> -Xylene	108-38-3
<i>o</i> -Xylene	95-47-6
<i>p</i> -Xylene	106-42-3
2,4-Xylenol	105-67-9
Zinc	7440-66-6
<u>Chlorinated solvent</u>	
Bis(2-chloroethyl) ether	111-44-4
Carbon tetrachloride	56-23-5
Chlorobenzene	108-90-7
Chloroethane	75-00-3
Chloroform	67-66-3
1,2-Dichlorobenzene	95-50-1
Dichlorodifluoromethane	75-71-8
1,1-Dichloroethane	75-34-3
1,2-Dichloroethane	107-06-2
<i>trans</i> -1,2-Dichloroethene	156-60-5
Dichloromethane	75-09-2
1,2-Dichloropropane	78-87-5
Hexachlorobutadiene	87-68-3
1,1,2,2-Tetrachloroethane	79-34-5
Tetrachloroethene	127-18-4
1,2,4-Trichlorobenzene	120-82-1
1,1,1-Trichloroethane	71-55-6
1,1,2-Trichloroethane	79-00-5
Trichloroethene	79-01-6
Trichlorofluoromethane	75-69-4
<u>Chlorofluorocarbon/refrigerant manufacture</u>	
Chloroform	67-66-3
Dibromochloromethane	124-48-1
Dichlorodifluoromethane	75-71-8
<i>trans</i> -1,2-Dichloroethene	156-60-5
Trichloroethene	79-01-6
Trichlorofluoromethane	75-69-4
Vinyl chloride	75-01-4

Table 16 - 75

<u>Substance</u>	<u>CAS RN</u>
<u>Hydrocarbon fuel or oils/manufacture/refining/by-product</u>	
Benz(e)acephenanthrylene	205-99-2
Benz[a]anthracene	56-55-3
Benzene	71-43-2
Benzo[a]pyrene	50-32-8
Carbon disulfide	75-15-0
Chloromethane	74-87-3
Chrysene	218-01-9
o-Cresol	95-48-7
Cyclohexane	110-82-7
Dibenz[a,h]anthracene	53-70-3
1,2-Dibromoethane	106-93-4
1,1-Dichloroethane	75-34-3
1,2-Dichloroethane	107-06-2
1,2-Dichloropropane	78-87-5
Ethanol	64-17-5
Ethylbenzene	100-41-4
Fluoranthene	206-44-0
Lead	7439-92-1
Methanol	67-56-1
Naphthalene	91-20-3
Nickel	7440-02-0
Nitrobenzene	98-95-3
Phenanthrene	85-01-8
Phenol	108-95-2
Toluene	108-88-3
1,2,4-Trichlorobenzene	120-82-1
m-Xylene	108-38-3
o-Xylene	95-47-6
p-Xylene	106-42-3
2,4-Xylenol	105-67-9
<u>Metal manufacture/treatment/degreasing</u>	
Arsenic	7440-38-2
Beryllium	7440-41-7
Cadmium	7440-43-9
Chromium	7440-47-3
Copper	7440-50-8
1,1-Dichloroethane	75-34-3
1,2-Dichloropropane	78-87-5
Hexachloroethane	67-72-1
Hydrogen cyanide	74-90-8
Lead	7439-92-1
Nickel	7440-02-0
Potassium cyanide	151-50-8
Selenium	7782-49-2
Silver	7440-22-4
Sodium cyanide	143-33-9
1,1,2,2-Tetrachloroethane	79-34-5
Tetrachloroethene	127-18-4
1,1,1-Trichloroethane	71-55-6
Trichloroethene	79-01-6

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Zinc

7440-66-6

<u>Substance</u>	<u>CAS RN</u>
<u>Organic solvent</u>	
Acetone	67-64-1
2-Butanone	78-93-3
Carbon disulfide	75-15-0
Cyclohexane	110-82-7
1,2-Dibromoethane	106-93-4
Dibutyl phthalate	84-74-2
Dimethyl sulfoxide	67-68-5
1,4-Dioxane	123-91-1
Ethylene glycol	107-21-1
Isophorone	78-59-1
Methanol	67-56-1
4-Methyl-2-pentanone	108-10-1
Nitrobenzene	98-95-3
Phenol	108-95-2
Quinoline	91-22-5
<i>m</i> -Xylene	108-38-3
<i>o</i> -Xylene	95-47-6
<i>p</i> -Xylene	106-42-3
<u>Pesticide/herbicide/fumigants (primary or manufacturing intermediate)</u>	
Aldrin	309-00-2
Bromomethane	74-83-9
Cadmium	7440-43-9
Carbon disulfide	75-15-0
Carbon tetrachloride	56-23-5
Chlordane	57-74-9
Chloroethane	75-00-3
Chloroform	67-66-3
Chloromethane	74-87-3
Copper	7440-50-8
<i>o</i> -Cresol	95-48-7
Cyclohexane	110-82-7
DDT	50-29-3
Dibromochloromethane	124-48-1
1,2-Dibromoethane	106-93-4
Dibutyl phthalate	84-74-2
1,2-Dichlorobenzene	95-50-1
1,3-Dichlorobenzene	541-73-1
1,4-Dichlorobenzene	106-46-7
2,4-Dichlorophenol	120-83-2
1,2-Dichloropropane	78-87-5
Dieldrin	60-57-1
Diethyl phthalate	84-66-2
2,4-Dinitrophenol	51-28-5
1,4-Dioxane	123-91-1
Endrin	72-20-8
Ethylene oxide	75-21-8
Hexachlorobenzene	118-74-1
$\gamma$ -Hexachlorocyclohexane	58-89-9

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<u>Substance</u>	<u>CAS RN</u>
Hydrogen cyanide	74-90-8
Isophorone	78-59-1
Naphthalene	91-20-3
N-Nitrosodiphenylamine	86-30-6
Pentachlorophenol	87-86-5
Silver	7440-22-4
1,1,2,2-Tetrachloroethane	79-34-5
Tetrachloroethene	127-18-4
Thallium	7440-28-0
Toxaphene	8001-35-2
1,2,4-Trichlorobenzene	120-82-1
1,1,1-Trichloroethane	71-55-6
1,1,2-Trichloroethane	79-00-5
2,4,6-Trichlorophenol	88-06-2
<i>m</i> -Xylene	108-38-3
<i>o</i> -Xylene	95-47-6
<i>p</i> -Xylene	106-42-3
2,4-Xylenol	105-67-9
<u>Pharmaceutical/medicine/disinfectant (primary or intermediate)</u>	
6-Chloro- <i>m</i> -cresol	59-50-7
Chloroform	67-66-3
<i>o</i> -Cresol	95-48-7
1,4-Dichlorobenzene	106-46-7
<i>trans</i> -1,2-Dichloroethene	156-60-5
Dichloromethane	75-09-2
Dimethyl sulfoxide	67-68-5
Ethanol	64-17-5
Ethylene glycol	107-21-1
Ethylene oxide	75-21-8
Hexachloroethane	67-72-1
Mercury	7439-97-6
Methanol	67-56-1
Nitrobenzene	98-95-3
Phenanthrene	85-01-8
Phenol	108-95-2
Quinoline	91-22-5
Tetrachloroethene	127-18-4
2,4-Xylenol	105-67-9
<u>Preservative</u>	
6-Chloro- <i>m</i> -cresol - glues, inks, leather, cosmetics	59-50-7
Chloroform - standard solutions	67-66-3
2,4-Dichlorophenol - wood	120-83-2
Dimethyl sulfoxide - cells at low temperature	67-68-5
2,4-Dinitrophenol - wood	51-28-5
Hexachlorobenzene - wood (starter for pentachlorophenol)	118-74-1
Pentachlorophenol - wood	87-86-5
2,4,6-Trichlorophenol - wood	88-06-2

<u>Substance</u>	<u>CAS RN</u>
<u>Other</u>	
Aroclor 1260 (PCB 1260) - electrical transformers	11096-82-5
Arsenic - glass, semiconductors	7440-38-2
Bromoform - mineral separation	75-25-2
Cadmium - batteries, solder, electronics	7440-43-9
Chloromethane - in cigarette smoke	74-87-3
Chromium - tanning, blood tracer, photography	7440-47-3
Chrysene - in cigarette smoke	218-01-9
Copper - plumbing, electrical conductors	7440-50-8
o-Cresol - ore flotation	95-48-7
1,4-Dichlorobenzene - air deodorizers	106-46-7
1,1-Dichloroethane - ore floatation	75-34-3
1,2-Dichloroethane - dry cleaning, soaps	107-06-2
trans-1,2-Dichloroethene - perfumes	156-60-5
Dichloromethane - photographic film	75-09-2
Diethyl phthalate - mosquito repellant	84-66-2
Dimethyl phthalate - insect repellant, perfumes	131-11-3
2,4-Dinitrophenol - photographic chemicals	51-28-5
2,4-Dinitrotoluene - explosives	121-14-2
2,6-Dinitrotoluene - explosives	606-20-2
1,4-Dioxane - cosmetics, scintillation counters	123-91-1
Dioxins (TCDD) - contaminant in prod. of chlorophenols	1746-01-6
Ethanol - alcoholic beverages, perfumes	64-17-5
Ethylene glycol - antifreeze	107-21-1
Ethylene oxide- rocket propellant	75-21-8
Fluoranthene - in cigarette smoke	206-44-0
Hexachlorobutadiene - heat-transfer fluid, hydraulics	87-68-3
Hexachloroethane - smoke candles and grenades	67-72-1
Hydrogen cyanide - gold and silver extraction from ore	74-90-8
Lead - construction material, storage batteries, solder	7439-92-1
Mercury - barometers, arc lamps, switches, dentistry	7439-97-6
Methanol - antifreeze	67-56-1
Naphthalene - lampblack, smokeless powder	91-20-3
Nickel - batteries, glass, ceramics	7440-02-0
Nitrobenzene - shoe and floor polish, leather dressings	98-95-3
Phenanthrene - explosives, dyestuffs	85-01-8
Potassium cyanide - extraction of ores	151-50-8
Selenium - photocells, rectifiers, photographic toner	7782-49-2
Silver - electrical conductors, dentistry	7440-22-4
Sodium cyanide - ore extraction	143-33-9
1,1,2,2-Tetrachloroethane - dry cleaning, in cement	79-34-5
Tetrachloroethene - dry cleaning	127-18-4
Thallium - infrared optical instruments, switches	7440-28-0
Toluene - explosives (TNT), scintillation counters	108-88-3
1,2,4-Trichlorobenzene - dye carrier	120-82-1
1,1,1-Trichloroethane - photographic film, dyeing	71-55-6
Trichlorofluoromethane - blowing agent for foams	75-69-4

## QUARTZ

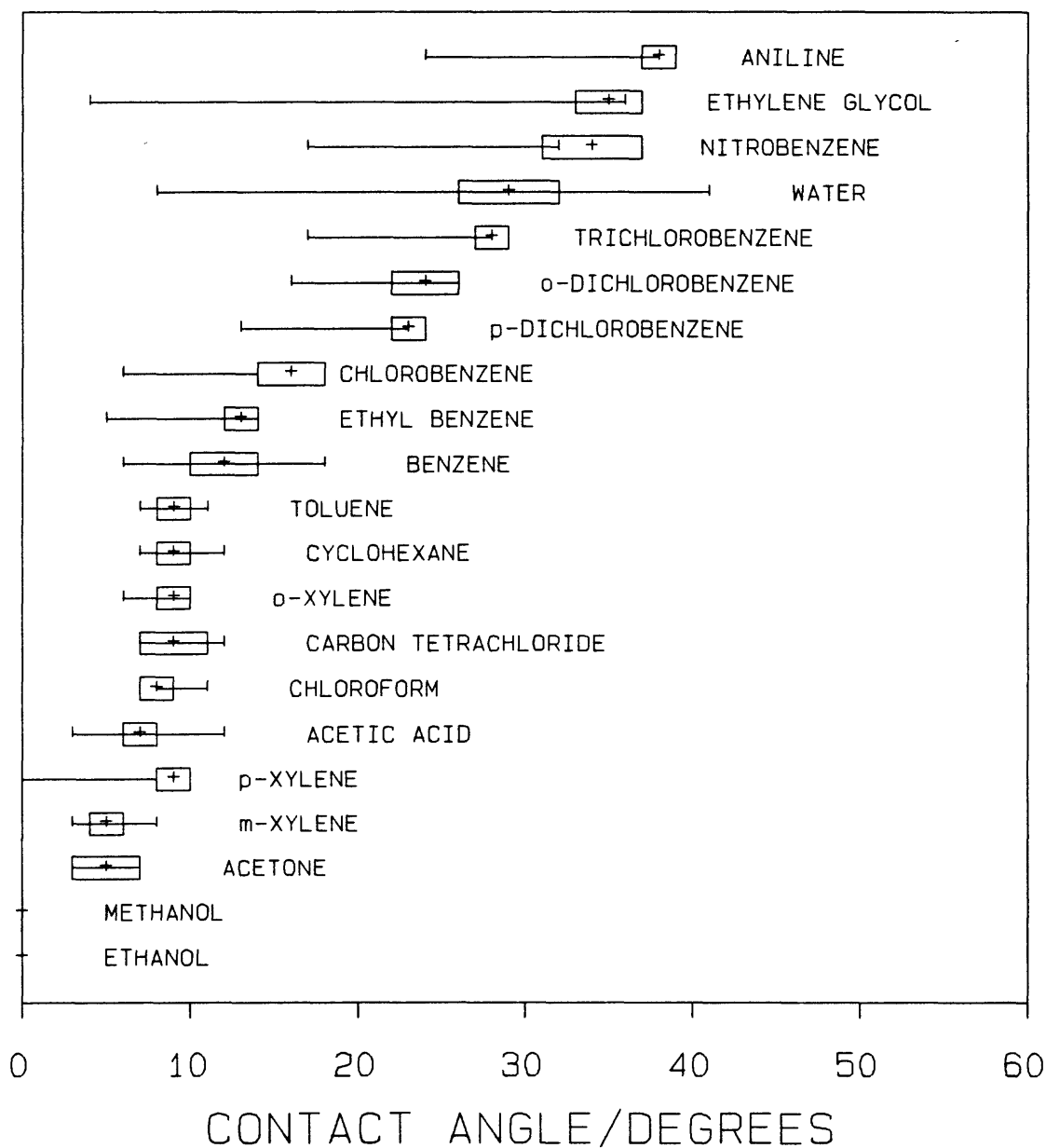


Figure 1. Contact angles of selected substances on quartz. The box represents the sessile drop angle (plus sign) plus or minus one standard deviation (limits of box). The range bar represents the receding angle (left end) and advancing angle (right end). Smaller angles indicate better wetting on a quartz substrate. From Ethington, 1990 [18].

# CALCITE

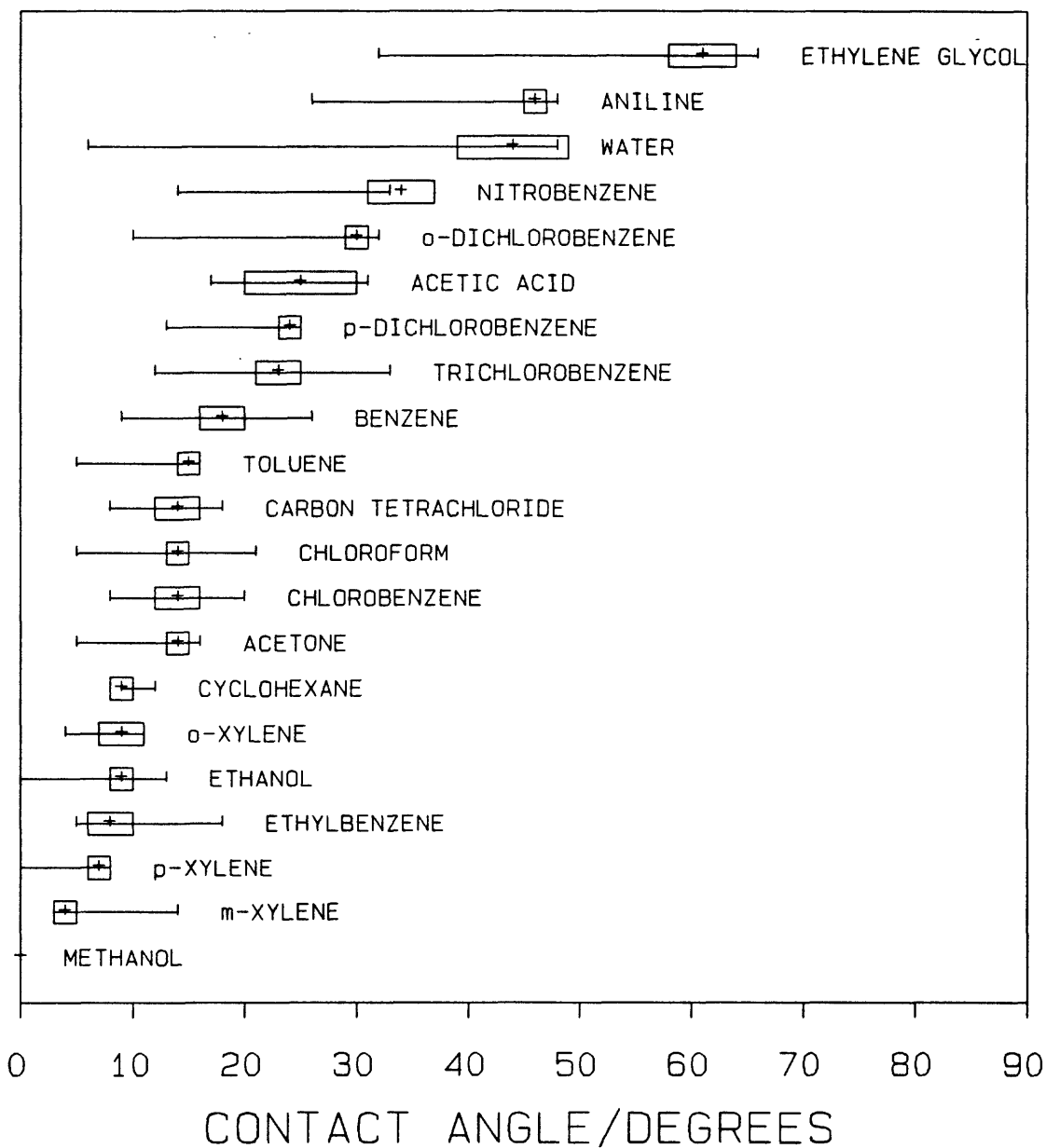


Figure 2. Contact angles of selected substances on calcite. The box represents the sessile drop angle (plus sign) plus or minus one standard deviation (limits of box). The range bar represents the receding angle (left end) and advancing angle (right end). Smaller angles indicate better wetting on a calcite substrate. From Ethington, 1990 [18].



## BIOTITE

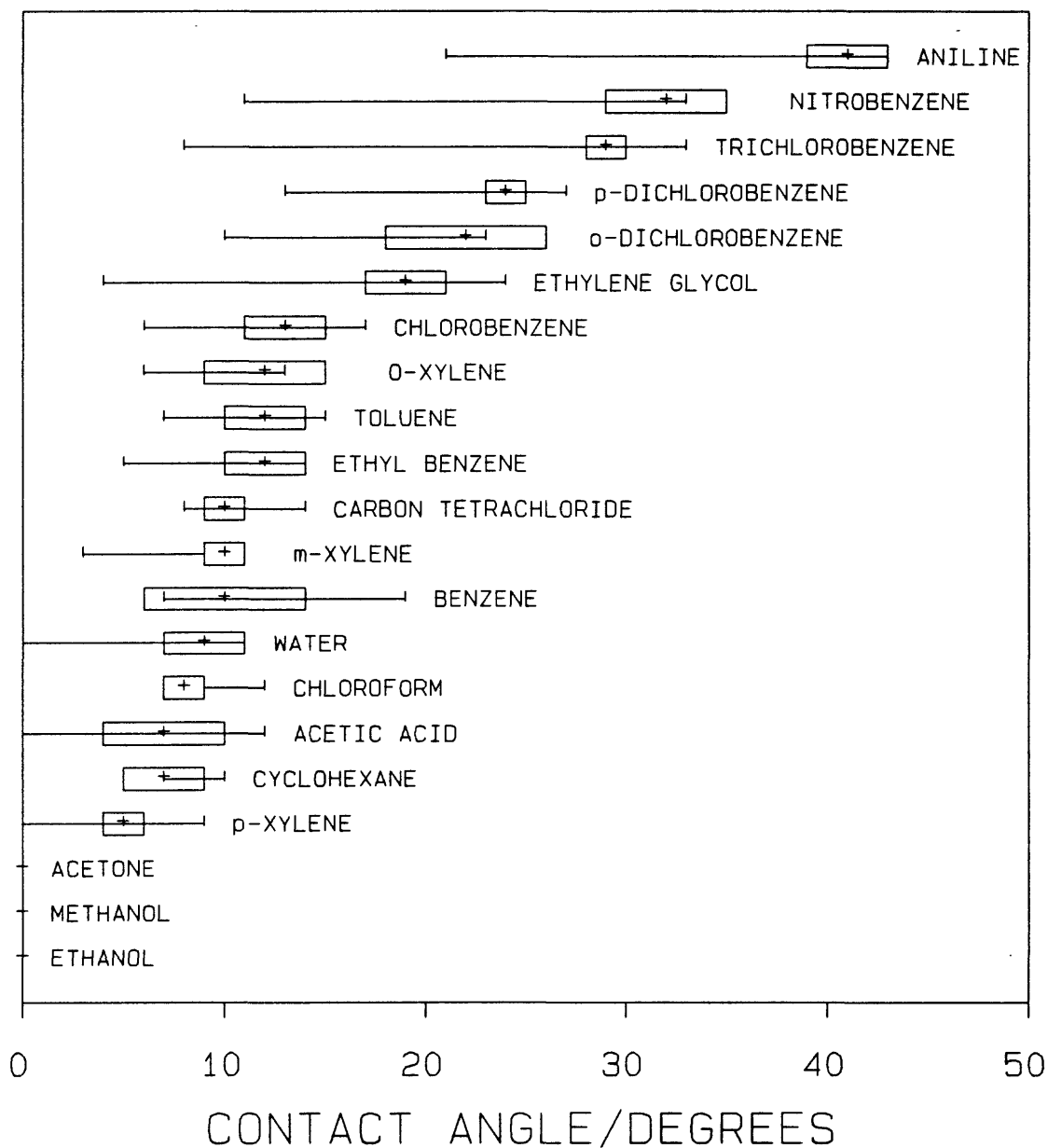


Figure 3. Contact angles of selected substances on biotite. The box represents the sessile drop angle (plus sign) plus or minus one standard deviation (limits of box). The range bar represents the receding angle (left end) and advancing angle (right end). Smaller angles indicate better wetting on a biotite substrate. From Ethington, 1990 [18].

## Ca-MONTMORILLONITE

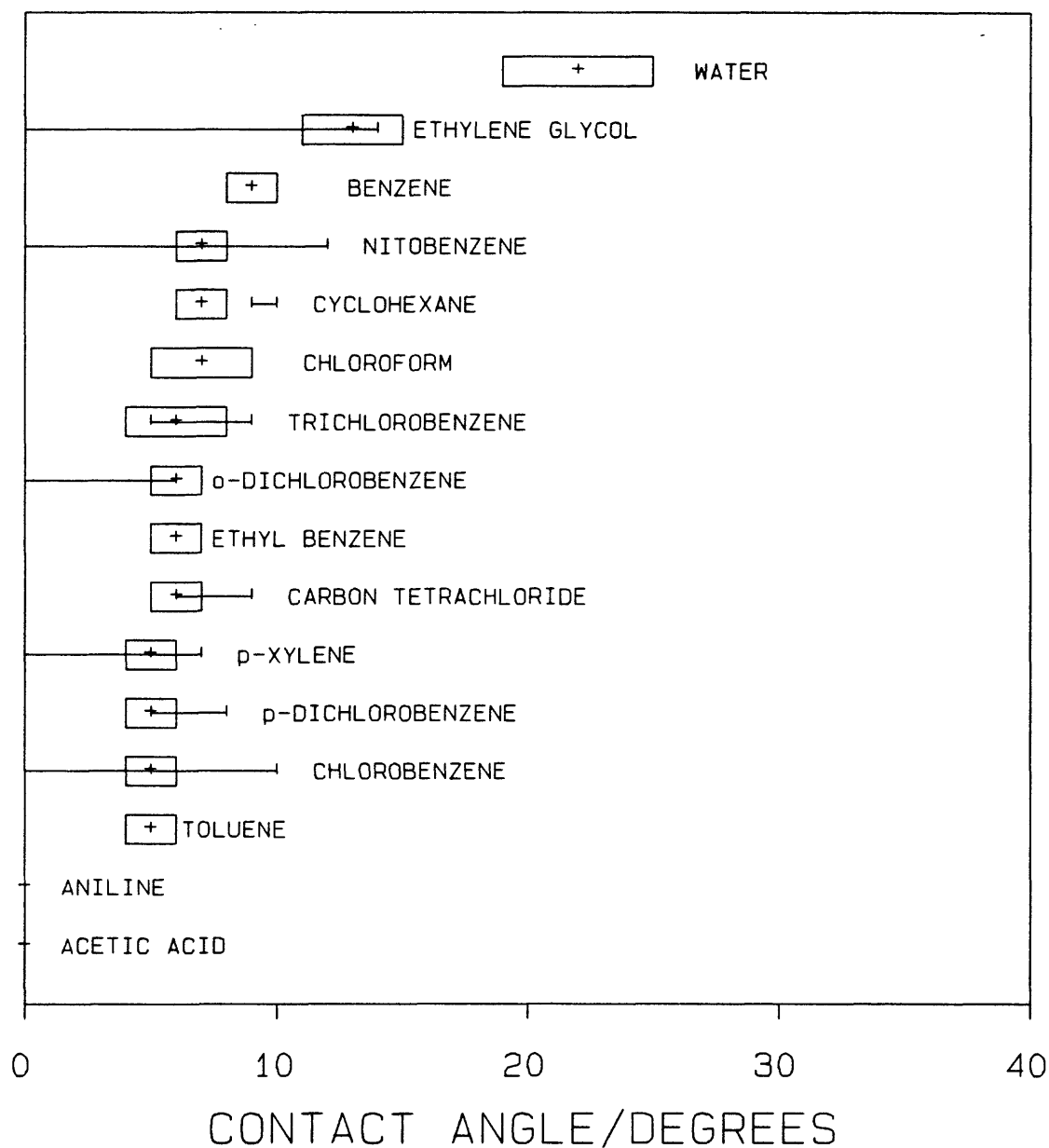


Figure 4. Contact angles of selected substances on Ca-montmorillonite. The box represents the sessile drop angle (plus sign) plus or minus one standard deviation (limits of box). The range bar represents the receding angle (left end) and advancing angle (right end). Smaller angles indicate better wetting on a Ca-montmorillonite substrate. From Ethington, 1990 [18].

## THE SUBSTANCES

For each substance, the data (when available in the literature) are given in the following categories and format. NA indicates that the property is not applicable to this substance considering the physical state at normal earth surface or near-surface conditions. Unknown indicates that the property for this substance was not found in this literature search. Subtopics in some categories were eliminated if nothing for that category was found (e.g. subtopics under Toxicity).

Name, Chemical formula, Chemical Abstract Service Registry Number

Synonyms

Molecular and/or structural formulas, Chemical family

Physical properties:

- Relative molecular mass
- Specific gravity
- Boiling point
- Melting point
- Refractive index
- Vapor pressure
- Vapor density
- Evaporation rate
- Relative dielectric permittivity
- Loss tangent
- Relaxation time
- Thermal conductivity
- Electrical resistivity
- Critical temperature
- Critical pressure
- Dynamic viscosity
- Kinematic viscosity
- Surface tension
- Contact angle
- Thermal expansion coefficient
- Compressibility
- Vapor diffusivity
- Solution diffusivity
- Electric dipole moment
- Ionization potential
- Magnetic volume susceptibility
- Speed of sound
- Heat of melting
- Heat of vaporization
- Heat of sublimation
- Heat capacity
- Heat of combustion
- Heat of formation
- Gibbs (free) energy

Analytical chemistry (partition coefficient, Henry's law constant, hydrolysis half-life, and ionization constant)

Electrochemical data

Clay-organic interaction data

Solubility

Form (color, state, odor, taste, commercial mixtures)

Use

Fire and explosion hazard (includes flash points and explosion limits)

Incompatibilities

Handling (includes personal protection methods and storage)

Health effects

Toxicity (includes exposure limits and carcinogenic potential)

Exposure (effects of external, oral, and inhalation exposures to humans)

## Acetic acid



CAS RN: 64-19-7

Syn: Acetic acid \* Ethanoic acid \* Ethylic acid \* Glacial acetic acid \*  
 Methane carboxylic acid \* Methylformic acid \* UN 2789 (DOT) \* UN 2790 (DOT)  
 \* Pyroligneous acid \* Vinegar acid \*

Molecular formula:  $\text{CH}_3\text{COOH}$ 

Carboxylic Acid

## Physical properties:

Relative molecular mass:	60.0526	
Specific gravity:	1.05	[32]
	1.051	[107]
	1.04955	[49]
	1.0492	[10], [105], [22], [106]
	1.049	[51], [104], [48], [47]
Boiling point:	118.1°C	[51], [104], [22]
	118.°C	[32], [48], [22]
	117.9°C	[10], [105], [107]
	117.885°C	[49]
Melting point:	16.7°C	[51], [107], [104], [48], [22]
	16.66°C	[49]
	16.63°C	[10], [22]
	16.604°C	[105]
	16.6°C	[32], [106]
Refractive index:	1.3720	[106]
	1.3719	[49]
	1.3716	[10], [105]
	1.3715	[22]
Vapor pressure:	0.666 kPa @ 6.3°C (5mm)	[20], [47]
	1.333 kPa @ 17.5°C (10mm)	[105], [20]
	1.520 @ 20°C (11.4mm)	[51], [104]
	1.467 @ 20°C (11mm)	[32]
	2.079 @ 25°C (15.6mm)	[49]
	2.666 @ 30°C (20mm)	[104]
Vapor density:	2.07	[51], [104]
	2.1	[32]
Evaporation rate:	0.97	[32]
Relative dielectric permittivity:	4.1 @ 2°C	[11]
	6.14 @ 20°C	[11]
	6.15 @ 20°C	[105], [10], [20]
	6.17 @ 20°C	[49]
	6.19 @ 25°C (1.5 MHz)	[2]
	6.29 @ 40°C	[105]
	6.3 @ 40°C	[11]
	6.6 @ 70°C	[11]
	6.62 @ 70°C	[105]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.177 W/(m-K) @ 0°C	[48]
	0.198 @ 12°C	[48]
	0.193 @ 20°C	[48]
	0.172 @ 20°C	[105]
	0.171 @ 20°C	[47]
	0.180 @ 25°C	[10], [48]

# 86 - Acetic acid

Electrical resistivity:	2.00 MOhm-m @ 0°C	[10], [11]	
	1.67 @ 25°C	[49]	
	0.893 @ 25°C	[10]	
	0.417 @ 25°C	[11]	
Critical temperature:	321.6°C	[105], [107]	
	321.3°C	[10]	
	319.56°C	[49]	
Critical pressure:	5.786 MPa	[49], [10], [105], [107]	
Dynamic viscosity:	1.314 mPa-s @ 15°C	[10]	
	1.30 @ 18°C	[105]	
	1.22 @ 20°C	[22]	
	1.155 @ 25.2°C	[105]	
	1.04 @ 30°C	[105]	
	1.00 @ 41°C	[105]	
	0.70 @ 59°C	[105]	
	0.60 @ 70°C	[105]	
	0.43 @ 100°C	[105]	
Kinematic viscosity:	1.252 μm²/s @ 15°C		
	1.24 @ 18°C		
	1.16 @ 20°C		
	1.101 @ 25.2°C		
	0.99 @ 30°C		
	0.95 @ 41°C		
	0.67 @ 59°C		
	0.57 @ 70°C		
	0.41 @ 100°C		
Surface tension:	28.8 mN/m @ 10°C vapor	[105]	
	27.42 @ 20°C	[49]	
	27.8 @ 20°C vapor	[105]	
	26.34 @ 30°C	[16], [49]	
	24.8 @ 50°C vapor	[105]	
Contact angle in degrees:	[18]		
	sessile	advancing	receding
quartz	6	12	3
calcite	22	31	17
biotite	7	10	0
Ca-mont.	0	5	0
Thermal expansion coefficient:	0.001078 K <sup>-1</sup> @ 20°C	[49]	
	0.00107 @ 20°C	[48]	
	0.00111 @ 55°C	[49]	
Compressibility:	0.875 nPa <sup>-1</sup> @ 15°C	[105]	
	0.908 @ 20°C	[105]	
	0.972 @ 30°C	[105]	
	1.037 @ 40°C	[105]	
	1.111 @ 50°C	[105]	
	1.191 @ 60°C	[105]	
	1.277 @ 70°C	[105]	
	1.368 @ 80°C	[105]	
Vapor diffusivity:	10.64 μm²/s @ 0°C	[47]	

Solution diffusivity:	3.31 nm <sup>2</sup> /s in Acetone	[47]
	2.11 in Benzene	[47]
	1.49 in CCl <sub>4</sub>	[47]
	0.13 in Ethylene glycol	[47]
	2.26 in Toluene	[47]
	1.24 in Water	[47]
Electric dipole moment:	5.804x10 <sup>-30</sup> C-m	[105], [10]
Ionization potential:	10.36 (PI)	[105]
Magnetic volume susceptibility:	-6.92x10 <sup>-6</sup> SI units @ 32°C	[105]
Speed of sound:	unknown	
Heat of melting:	11.723 kJ/mol	[10]
	11.72	[49]
	11.666	[48]
	11.535	[105]
Heat of vaporization:	41.717 kJ/mol	[105]
	39.718	[105]
	24.388	[48]
	24.37	[49]
	23.710	[10]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.1243 kJ/(mol-K) (liq)	[105], [10]
	0.1231 (liq)	[105], [49]
	0.0670 (gas)	[105]
	0.0666 (gas)	[105], [10]
Heat of combustion:	-875.1 kJ/mol @ 25°C (liq)	[105]
	-874.20 (liq)	[49]
Heat of formation:	-484.5 kJ/mol @ 25°C (liq)	[105], [10], [49]
	-435.1 (gas)	[10]
	-432.5 (gas)	[105]
	-432.25 (gas)	[49]
Gibbs (free) energy:	-390.2 kJ/mol @ 25°C (liq)	[105], [10]
	-376.9 (gas)	[10]
	-374.3 (gas)	[105]
Analytical chemistry:	pP <sub>oct</sub> = -0.31	[104], [21]
	-0.17	[104], [21]
	pK <sub>s</sub> = 1.5	[10]
	14.45	[10], [49]
	pK <sub>a</sub> = 4.78 @ 0°C	[11]
	4.76 @ 20°-35°C in water	[10], [11]
	4.7560 @ 25°C in water	[10], [49]
	9.52 in methanol	[10]
	10.32 in ethanol	[10]
	11.4 in dimethyl sulfoxide	[10]
	9.75 in acetone+10% water	[10]
	pK <sub>BH</sub> = unknown	
Henry's law constant =	1.x10 <sup>-5</sup> kPa-m <sup>3</sup> /mol @ pH=4	
	to 1.x10 <sup>-7</sup> @ pH=7	[24]
Hydrolysis half-life =	unknown	

Electrochemical data: Kolthoff and Reddy (1961), Mather (1961), Spritzer et al. (1965), Tsuji and Elving (1969), Meites and Zuman (1977)

## 88 - Acetic acid

**Clay-organic interaction data:** Acetic acid increases the hydraulic conductivity of silicate grouted soil (Lord et al., 1983). Carbonyl stretching frequency of acetic acid in the unadsorbed phase and when adsorbed in montmorillonite. Basal spacings of montmorillonite complexes with acetic acid. New interlayer complexes of halloysite with acetic acid. (Theng, 1974). Also see Larson and Sherman (1964), Brindley and Moll (1965), and Carr and Chih (1971).

**Solubility:** Soluble in carbon disulfide. Miscible with water, ethanol, ether, acetone, and benzene, n-heptane, carbon tetrachloride. Insoluble in carbon disulfide. [10],[47],[105]

**Form:** Colorless liquid or solid. Pungent vinegar-like odor. Glacial acetic acid is the pure form containing 99.8% minimum. Usually water solutions are known as acetic acid. [22],[56]

**Use:** In production of acetic anhydride for cellulose acetate, fibers, plastics, and aspirin; in production of vinyl acetate for polymers, coatings, and adhesives; in production of acetic esters for solvents in plastics, coatings, and pharmaceutical industries; in chemical industries as an esterifying agent, acetylating agent, solvent, and reaction medium; as an acidifying and neutralizing agent; in food canning industries as a food additive (preservative) or flavorant for pickles, fish, meat, candy, and glazes; in textile and dye industries as a solvent, acidifying and neutralizing agent, intermediate in production of dyestuffs, dye catalysts, textile finishing, dye after-treatment, and production of nylon and acrylic fibers. Acetic acid occurs in both plants and animals as normal metabolite. [22],[32],[56]

**Fire and explosion hazard:** Moderate.

Flash point: (CC) 43°C [51]  
(CC) 40°C [32],[107]  
(CC) 42°C [49]  
(OC) 44.4°C [107]  
(OC) 44°C [49]  
(OC) 43.3°C [22]  
uel: 16.0% @ 100°C [51],[32]  
lel: 5.4% @ 100°C [51],[32]  
Autoign. temp.: 465°C [51]  
427°C [107],[22]

Combustible, corrosive liquid. Moderate fire and explosion hazard when exposed to heat, sparks or flame. Dangerous, as toxic gases and vapors (such as carbon monoxide and carbon dioxide) may be released in a fire. Can react vigorously with oxidizing materials. Fight fire with CO<sub>2</sub>, dry chemical, alcohol or polymer foam or water spray. [32],[51],[107],[55]

**Incompatibility:** Strong oxidizers; strong bases; chromic acid; 5-azidotetrazole; hydrogen peroxide; sodium peroxide; nitric acid; acetaldehyde; 2-amino-ethanol; NH<sub>4</sub>NO<sub>3</sub>; BrF<sub>5</sub>; ClF; chlorosulfonic acid; (O<sub>3</sub>+diallyl methyl carbinol); ethylenediamine; ethylene imine; H<sub>2</sub>O<sub>2</sub>; (HNO<sub>3</sub>+acetone); potassium-tert-butoxide; oleum; HClO<sub>4</sub>; permanganates; P(OCN)<sub>3</sub>; PCl<sub>3</sub>; KOH; NaOH; *m*-xylene. Excellent solvent for many synthetic resins or rubber. Attacks most common metals, including most stainless steels. [51],[32],[107],[56],[55]



**Handling:** Avoid heat, sources of ignition and flame. Prevent skin contact or inhalation (leather, neoprene, latex or nitrile gloves; lab coat and apron, safety goggles, face shield, body shield). Use appropriate respirator to avoid inhalation. Use in well-ventilated area (fume hood). Wash contaminated clothing before reuse. Discard contaminated shoes. Safety shower and eyebath should be available. Keep container tightly closed. Store in cool, dry well-ventilated flammable liquid storage area or cabinet. [32],[56],[107],[53],[55]

**Health effects:** Acetic acid is corrosive and an irritant. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include respiratory system, mucous membranes, skin, eyes, and teeth. The vapor is a severe irritant to the eyes, mucous membranes, and the skin. It attacks the skin easily and can cause dermatitis, ulcers, and severe eye damage which may be followed by loss of sight. Flush immediately in case of contact with eyes or skin. Inhalation of concentrated vapors may cause serious damage to the lining of the nose, throat, and lungs and result in spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. Swallowing concentrated solutions may cause severe injury or death. [32],[51],[56],[107],[55]

**Toxicity:** Moderate.

TWA: 10 ppm (25 mg/m<sup>3</sup>) [1]  
 STEL: 15 ppm (37 mg/m<sup>3</sup>) [1]  
 CL: unknown  
 IDLH: 1000 ppm (2450 mg/m<sup>3</sup>) [107],[56]  
 Peak: 40 ppm (100 mg/m<sup>3</sup>) for 5 min [107]  
 Odor threshold: 0.2-24 ppm (0.5-60 mg/m<sup>3</sup>) [32]  
                   10 ppm (25 mg/m<sup>3</sup>) [107]  
 Carcinogenicity: none [104]  
 Mutagenicity: none [104]

**Exposure:**

External:

Non-lethal: 50 mg/24 hr -- mild skin irritation [51],[55]  
             10-12 ppm (25-30 mg/m<sup>3</sup>) -- nasal irritation [32]  
             >25 ppm (60 mg/m<sup>3</sup>) -- extreme eye and nasal irritation [32]  
             80-200 ppm (200-500 mg/m<sup>3</sup>) for 7-12 years -- acclimatized workers have experienced blackening and hyperkeratosis of the skin of the hands, conjunctivitis (but no corneal damage), bronchitis and pharyngitis, and erosion of the exposed teeth [32]

Lethal: unknown

Oral:

Non-lethal: 1.47 mg/kg body wt -- gastrointestinal effects [51]  
 Lethal: 308 mg/kg body wt -- death of an adult male [51]

Inhalation:

Short-term Inhalation Limits: 40 ppm (100 mg/m<sup>3</sup>) for 5 min [107]  
 Non-lethal: 50 ppm (125 mg/m<sup>3</sup>) -- intolerable to most persons [32]  
             200 ppm (500 mg/m<sup>3</sup>) for 60 min -- severe toxic effects [32]  
             816 ppm (2000 mg/m<sup>3</sup>) for 3 min -- systemic irritation [51]

Lethal: unknown

## 90 - Acetone

Acetone

 $C_3H_6O$ 

CAS RN: 67-64-1

Syn: Acetone \* 2-Propanone \* Chevron acetone \* Dimethylformaldehyde \*  
 Dimethylketal \* Dimethyl ketone \* DMK \* Ketone propane \*  $\beta$ -Ketopropane \*  
 Methyl ketone \* Propanone \* Pyroacetic acid \* Pyroacetic ether \* RCRA Waste  
 Number U002 \* UN 1090 (DOT) \*

Molecular formula:  $CH_3-CO-CH_3$ 

Aliphatic Ketone

## Physical properties:

Relative molecular mass:	58.080	
Specific gravity:	0.792	[22], [47]
	0.791	[107], [104], [48]
	0.7908	[10]
	0.78998	[49]
	0.7899	[105], [106]
Boiling point:	56.5°C	[47], [108]
	56.48°C	[51]
	56.24°C	[10]
	56.2°C	[105], [104], [22]
	56.1°C	[107], [48]
	56.067°C	[49]
Melting point:	-94.0°C	[108]
	-94.3°C	[48], [22]
	-94.6°C	[51], [47]
	-94.7°C	[107], [49]
	-95.°C	[104]
	-95.3°C	[106]
Refractive index:	-95.35°C	[10], [105]
	1.3591	[22], [108]
	1.3588	[105], [10], [106]
	1.35868	[49]
Vapor pressure:	5.333 kPa @ -9.4°C (40mm)	[105], [47]
	8.00 @ -2°C (60mm)	[47]
	11.9 @ 5°C (89mm)	[104]
	13.33 @ 7.7°C (100mm)	[105], [47]
	24.227 @ 20°C (181.72mm)	[49]
	26.66 @ 22.7°C (200mm)	[47]
	30.806 @ 25°C (231.06mm)	[49]
	36.00 @ 30°C (270mm)	[104]
	53.33 @ 39.5°C (400mm)	[51], [105]
Vapor density:	2.00	[51], [107], [104]
Evaporation rate:	5.59	[49]
Relative dielectric permittivity:	25.91 @ -20°C	[11]
	23.65 @ 0°C	[11]
	21.45 @ 20°C	[11]
	21.248 @ 20°C	[2]
	20.9 @ 20°C	[49]
	20.56 @ 25°C	[49]
	20.7 @ 25°C	[105], [10], [11]
	20.68 @ 25°C	[2]
	20.20 @ 30°C	[49]
	20.069 @ 30°C	[2]
	19.38 @ 40°C	[11]

	18.965 @ 40°C	[2]	
	17.7 @ 56°C	[105]	
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	0.177 W/(m-K) @ -20°C	[20]	
	0.169 @ 0°C	[20]	
	0.177 @ 0°C	[10]	
	0.184 @ 0°C	[48]	
	0.1902 @ 16°C	[105]	
	0.162 @ 20°C	[20]	
	0.180 @ 20°C	[48]	
	0.1765 @ 30°C	[47]	
	0.155 @ 40°C	[20]	
Electrical resistivity:	9.1 MOhm-m @ -15°C	[11]	
	0.1667 @ 0°C	[11]	
	0.5 @ 18°C	[10], [11]	
	0.1667 @ 25°C	[10]	
Critical temperature:	236.5°C	[10]	
	235.5°C	[105]	
	235.0°C	[47]	
	234.95°C	[49]	
Critical pressure:	4.783 MPa	[10]	
	4.76	[105], [47]	
	4.696	[49]	
Dynamic viscosity:	0.450 mPa-s @ -10°C	[105]	
	0.399 @ 0°C	[105], [48]	
	0.362 @ 10°C	[48]	
	0.337 @ 15°C	[105], [10], [48]	
	0.331 @ 20°C	[48]	
	0.316 @ 25°C	[105], [48]	
	0.295 @ 30°C	[105], [48]	
	0.280 @ 41°C	[105]	
Kinematic viscosity:	0.569 μm²/s @ -10°C		
	0.505 @ 0°C		
	0.458 @ 10°C		
	0.427 @ 15°C		
	0.418 @ 20°C		
	0.400 @ 25°C		
	0.373 @ 30°C		
	0.354 @ 41°C		
Surface tension:	26.21 mN/m @ 0°C air, vapor	[105]	
	23.70 @ 20°C air, vapor	[105]	
	23.32 @ 20°C	[49]	
	22.68 @ 25°C	[49]	
	22.01 @ 30°C	[49]	
	21.16 @ 40°C air, vapor	[105]	
Contact angle: [18]			
	sessile	advancing	receding
quartz	6	NA	NA
calcite	11	16	6
biotite	7	0	0
Ca-mont.	swelled	swelled	swelled

## 92 - Acetone

Thermal expansion coefficient:	0.0135 K <sup>-1</sup> @ 10°C	[48]
	0.001375 @ 20°C	[48]
	0.00143 @ 20°C	[49], [48]
	0.001433 @ 30°C	[48]
	0.001463 @ 40°C	[48]
Compressibility:	1.229 nPa <sup>-1</sup> @ 20°C	[105]
	1.269 @ 20°C	[49]
	1.324 @ 25°C	[49]
	1.334 @ 30°C	[105]
	1.464 @ 40°C	[105]
Vapor diffusivity:	10.9 μm <sup>2</sup> /s @ 0°C	[47]
Solution diffusivity:	unknown	
Electric dipole moment:	9.61x10 <sup>-30</sup> C-m	[10], [105]
	8.97x10 <sup>-30</sup>	[49]
Ionization potential:	9.69 eV (PI)	[105]
Magnetic volume susceptibility:	-5.78x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	1203. m/s @ 20°C	[20]
	1174. @ 25°C	[105]
	1158. @ 30.5°C	[20]
	1097. @ 41°C	[20]
Heat of melting:	5.719 kJ/mol	[10]
	5.691	[105]
	5.69	[49]
	5.5913	[48]
Heat of vaporization:	31.993 kJ/mol	[105]
	30.396	[48]
	29.11	[10]
	29.09	[49]
	31.3 @ 25°C	[49]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.1264 kJ/(mol-K) (liq)	[10], [105]
	0.1249 (liq)	[49]
	0.0753 (gas)	[105]
	0.0749 (gas)	[10]
@ 20°C:	0.1255 (liq)	[48]
Heat of combustion:	-1791. kJ/mol @ 25°C (liq)	[105]
	-1789.79 (liq)	[49]
	-1821.38 (gas)	[49]
Heat of formation:	-247.8 kJ/mol @ 25°C (liq)	[10]
	-246.81 (liq)	[49]
	-217.15 (gas)	[49]
	-216.7 (gas)	[10]
Gibbs (free) energy:	-155.8 kJ/mol @ 25°C (liq)	[10]
	-153.1 (gas)	[10]
Analytical chemistry:	pP <sub>oct</sub> = -0.24	[104], [21]
	pK <sub>s</sub> = 32.5	[49]
	pK <sub>a</sub> = 24.2	[49]
	pK <sub>BH</sub> = -2.85 in aqueous H <sub>2</sub> SO <sub>4</sub>	[49]
Henry's law constant =	0.00372 kPa-m <sup>3</sup> /mol	[24]
	0.00402 @ 25°C	[41]
Hydrolysis half-life =	unknown	

**Electrochemical data:** Baizer (1983), Feoktistov (1983), Heyrovsky (1962), Meites and Zuman (1977), Meites et al. (1982)

**Clay-organic interaction data:** Acetone increases the hydraulic conductivity of silicated grouted and clay soils (Anderson and Brown, 1981; Brown and Thomas, 1984; Brown et al., 1983, 1986; Lord et al., 1983). Isotherm and X-ray diffraction data for the adsorption of acetone by montmorillonite saturated with different cations. Complex swelling behavior of Ca-montmorillonite in water-acetone mixtures (see also [18]). Basal spacings of montmorillonite samples containing  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$  and increasing proportions of  $\text{Li}^+$  after heat treatment to 493 K for 24 hours and solvation by acetone. Carbonyl stretching frequency of acetone in the unadsorbed phase and when adsorbed in montmorillonite. C=O stretching frequencies of acetone adsorbed by trimethylammonium and tetramethylammonium montmorillonite. Interlayer complexes of halloysite with acetone. Interaction energies for cation-acetone dipole systems. Complexes formed with rehydrated halloysite obtained by washing the potassium acetate complex with water. Infra-red spectra of Ca- and Mg-montmorillonite and their complexes with acetone under various conditions. Infra-red band frequencies, basal spacings and retention data for complexes between montmorillonite containing different interlayer cations and acetone (Theng, 1974). Also see Acar et al., 1984, 1985; Anderson and Brown, 1981; Barshad, 1952; Bissada et al., 1967; Brindley et al., 1969; Brown and Thomas, 1984; Brown et al., 1983, 1984; 1986; Carr and Chih, 1971; Griffin et al., 1984; Glaeser, 1948; Lord et al., 1983; Mortland, 1970; Ruiz-Amil, 1957.

**Solubility:** Miscible with water, ethanol, ether, benzene, chloroform, dimethylformaldehyde, most oils. [105],[51],[22],[108]

**Form:** Colorless liquid. Fragrant, characteristic mint-like odor. Pungent, sweetish taste. Technical and reagent grades are 99.5% pure with 0.5% water. [107]

**Use:** Solvent for fats, oils, waxes, resins, nitrocellulose, cellulose, acetylene, paint, varnish, lacquer and many other substances; organic chemical manufacturing; dyestuffs; sealants and adhesives; storing acetylene gas; cleaning and drying of precision equipment; purifying paraffin; hardening and dehydrating tissues; specification testing of vulcanized rubber products; smokeless powder manufacture; nail polish remover. Acetone is a normal microcomponent in blood and urine. Acetone is also present in cigarette smoke (1100 ppm) and gasoline exhaust (2.3 - 14 ppm) and commonly occurs in sanitary landfill leachate. [104],[56],[5]

**Fire and explosion hazard:** Very high.

Flash point: (CC) -18°C [51],[107],[108]  
                   (CC) -17°C [49]  
                   (OC) -9°C [49]  
                   (OC) -15.6°C [107]

uel: 12.8% [51],[107],[22]  
       13.0% [10]

lel: 2.6% [51],[107],[22]  
       2.5% [10]

Autoign. temp.: 465°C [51],[107]

## 94 - Acetone

Volatile and extremely flammable liquid. Dangerous fire hazard when exposed to heat, sparks, flame or oxidizers. Moderate explosion hazard when vapor exposed to flame. Flashback along vapor trail may occur. Fight fire with CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. Water should not be used as it will scatter and spread fire. [51],[107]

**Incompatibility:** Chloroform; (CHCl<sub>3</sub> + a base); CrO; Cr(OC<sub>2</sub>H<sub>5</sub>)<sub>2</sub>; (nitric + acetic acid); NOCl; nitrosyl perchlorate; nitryl perchlorate; permonosulfuric acid; potassium tertbutoxide; NaOBr; (sulfuric acid + potassium dichromate); (thiodiglycol + hydrogen peroxide); H<sub>2</sub>O<sub>5</sub>S; trichloromelamine; bromoform; HNO<sub>3</sub>; activated C; H<sub>2</sub>SO<sub>4</sub>; BF<sub>3</sub>; Br<sub>2</sub>; chromyl chloride; H<sub>2</sub>O<sub>2</sub>; F<sub>2</sub>O<sub>2</sub>; SCl<sub>2</sub>; thiotrithiaxyl perchlorate; strong oxidizing agents; acids. [51],[56]

**Handling:** Keep away from heat, sparks and flame. Avoid prolonged skin contact or inhalation (rubber, latex or neoprene gloves; lab coat, chemical safety goggles, face shield). Use in well-ventilated area (fume hood, appropriate respirator). Safety shower and eye bath should be available. Keep container tightly closed. Store in cool, dry, well-ventilated, flammable liquid storage area. [53],[51]

**Health effects:** Acetone can be an irritant. Routes of entry are inhalation, ingestion, and skin or eye contact. Points of attack include the respiratory system and skin. Prolonged or repeated topical use of acetone may cause erythema, dryness. Inhalation may produce headache, fatigue, excitement, bronchial and/or upper respiratory tract irritation, and, in large amounts, narcosis. It can cause severe eye irritation. Serious poisonings are rare. A food additive permitted for human consumption. A common air contaminant. [51],[60]

### **Toxicity:** Low

TWA: 750 ppm (1780 mg/m<sup>3</sup>) [1]

STEL: 1000 ppm (2375 mg/m<sup>3</sup>) [1]

CL: unknown

IDLH: 20000 ppm (47,500 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 100 ppm (235 mg/m<sup>3</sup>) [107]

0.5-500 ppm (1-1000 mg/m<sup>3</sup>) [104]

Carcinogenicity: none [104]

Mutagenicity: none [104]

**Exposure:**

**External:**

Non-lethal: 500 ppm (1185 mg/m<sup>3</sup>) -- eye irritation [51],[55]

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: 50 mL (estimated) [104]

1159 mg/kg body wt -- death of an adult human [55]

**Inhalation:**

Short-term Inhalation Limits: 1000 ppm (2375 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: 400 ppm for 60 min -- unsatisfactory conditions begin [104]

800 ppm for 60 min -- symptoms of illness appear [104]

4000 ppm for 60 min -- severe toxic effects [51]

12000 ppm (28,500 mg/m<sup>3</sup>) -- CNS effects [51]

25-920 ppm repeatedly -- chronic conjunctivitis, pharyngitis,  
bronchitis, gastritis, gastro-duodenitis [104]

0.2 ppm (0.440 mg/m<sup>3</sup>) for 6 min [51]

4.2 ppm (10 mg/m<sup>3</sup>) for 6 hr [51]

Lethal: unknown

## 96 - Acrolein

Acrolein

 $C_3H_4O$ 

CAS RN: 107-02-8

Syn: Acrolein \* 2-Propenal \* Acquinite \* Acraldehyde \* *trans*-Acrolein \* Acrolein, inhibited \* Acrylaldehyde \* Acrylic aldehyde \* Allyl aldehyde \* Aqualin \* Aqualine \* Biocide \* Crolean \* Ethylene aldehyde \* Magnacide \* Magnacide H \* NSC 8819 \* Propenal \* Prop-2-en-1-al \* 2-Propen-1-one \* Propylene aldehyde \* RCRA Waste Number P003 \* Slimicide \* UN 1092 (DOT) \*

Molecular formula:  $CH_2=CH-CHO$ 

Unsaturated Aldehyde

## Physical properties:

Relative molecular mass:	56.0642	
Specific gravity:	0.843	[107]
	0.841	[10], [105], [51], [47], [106]
	0.84	[32]
	0.8389	[49], [10]
Boiling point:	53.°C	[56], [107]
	52.7°C	[10], [22]
	52.69°C	[49]
	52.5°C	[104], [51], [47]
	52.5°-53.5°C	[105]
	52.°-53°C	[106]
	51.7°C	[32]
Melting point:	-86.9°C	[106]
	-86.95°C	[49], [105]
	-87.0°C	[10], [107], [22], [32]
	-87.7°C	[104], [51], [47]
Refractive index:	1.4017	[49], [10], [105], [106]
Vapor pressure:	5.333 kPa @ -15°C (40mm)	[105], [47]
	8.00 @ -7.5°C (60mm)	[47]
	13.332 @ 2.5°C (100mm)	[105], [47]
	26.67 @ 17.5°C (200mm)	[47]
	28.53 @ 20°C (214mm)	[32]
	29.33 @ 20°C (220mm)	[104]
	35.33 @ 25°C (265mm)	[49], [23]
	44.00 @ 30°C (330mm)	[104]
	53.329 @ 34.5°C (400mm)	[105], [47]
Vapor density:	1.94	[104], [107], [51]
	1.94 @ bp	[32]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	0.0645 MOhm-m	[49]
Critical temperature:	254.°C	[107]
Critical pressure:	5.08 MPa	[107]
Dynamic viscosity:	unknown	
Kinematic viscosity:	unknown	
Surface tension:	24.0 mN/m @ 20°C	[107]
Contact angle:	unknown	
Thermal expansion coefficient:	NA	
Compressibility:	unknown	
Vapor diffusivity:	unknown	



Solution diffusivity:	unknown	
Electric dipole moment:	10.41x10 <sup>-30</sup> C-m	[105]
	9.67x10 <sup>-30</sup> C-m @ 20°C	[49],[10]
Ionization potential:	10.10 eV (PI)	[105]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	31.940 kJ/mol	[105]
	28.33	[49]
	28.16	[107]
Heat of sublimation:	unknown	
Heat capacity @ 17°-44°C:	0.11987 kJ/(mol-K) (liq)	[49]
Heat of combustion:	-1634.7 kJ/mol @ 25°C (liq)	[49]
	-1631.2 @ 20°C (liq)	[105]
Heat of formation:	-117.1 kJ/mol @ 25°C (liq)	[10]
	-85.83 (gas)	[10]
Gibbs (free) energy:	-67.70 kJ/mol @ 25°C (liq)	[10]
	-64.69 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	0.01	[31]
	-0.09	[8]
	-0.10	[23]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	0.000446 kPa-m <sup>3</sup> /mol @ 25°C	[41]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Meites et al. (1977a), Meites et al. (1977b), Meites et al. (1982)

Clay-organic interaction data: Theng (1974) reports polymer formation upon adsorption.

Solubility: Soluble in water, ethanol, ether, acetone, benzene. [10],[105]  
 20.8 wt% in water @ 20°C [104],[49]  
 22. wt% in water @ 20°C [32]  
 40. wt% in water [10],[47]

Form: Colorless or light yellow liquid. Piercing, disagreeable, choking, extremely irritating, pungent odor. Technical grades contain 0.1% hydroquinone (or hydroquinone) to inhibit polymerization. Industrial grades may be only 92% pure. [104],[22],[107],[22].

Use: Primary use is as an intermediate in the production of glycerine and methionine analogs (poultry feed protein supplements). Chemical synthesis 1,2,6-hexanetriol, glutaraldehydes, acrylates, polyurethane foams, polyester resins, methionine; liquid fuel; antimicrobial agent; herbicide in algae and aquatic weed control; slimicide in paper manufacture; tear gas; denaturant in alcohol. Present in cigarette smoke (150 ppm) and automobile exhaust (0.2-5.3 ppm). [56],[104],[22],[32]

## 98 - Acrolein

**Fire and explosion hazard:** High.

Flash point: (CC) -25°C [107]

(CC) -26°C [32]

(OC) <-17.78°C [51],[107],[49],[22]

uel: 31% [51],[107],[22],[32]

lel: 2.8% [51],[107],[22],[32]

Autoign. temp.: 235°C [51],[107],[32]

278°C [22]

Extremely flammable liquid. Dangerous fire hazard when exposed to heat, flame or oxidizers. Dangerous explosion hazard when exposed to incompatible substances. Emits highly toxic fumes when heated to decomposition. Can react vigorously with oxidizing materials. Flashback along vapor trail may occur. Polymerizes near 200°C. Fight fire with CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. Water may be ineffective on fire. Cool exposed containers with water. [51],[107],[32],[55]

**Incompatibility:** Acids; oxidizers; reducing agents; oxygen; alkalis; amines; SO<sub>2</sub>; thiourea; metal salts; oxidants; ammonia; (light + heat).

Undergoes uncatalyzed polymerization reaction around 200°C. Light promotes polymerization. [51],[107],[56],[55]

**Handling:** Avoid heat, flame, and sources of ignition. Do not inhale mist or vapor (appropriate respirator or self-contained breathing apparatus required). Wear protective clothing to prevent any skin contact (CPE or Chloropel® suit and gloves; splash-proof chemical goggles). Readily absorbed through skin. Facilities for eye wash and quick body drenching should be available. Keep container tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet. Store in secure poison area. [53],[56],[32],[55]

**Health effects:** Acrolein is an intense irritant. Routes of entry are inhalation, ingestion, and eye and skin contact. Points of attack include the heart, lungs, eyes, skin, and respiratory system. It is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. It may cause first degree burns after short exposure and second degree burns after longer exposure. Symptoms of overexposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. It may cause an allergic skin reaction. [51],[107],[56],[32],[55]

**Toxicity:** High.

TWA: 0.1 ppm (0.25 mg/m<sup>3</sup>) [1]

STEL: 0.3 ppm (0.8 mg/m<sup>3</sup>) [1]

CL: unknown

IDLH: 5.0 ppm (11.5 mg/m<sup>3</sup>) [56],[107]

Peak: unknown

Odor threshold: 0.2-2.0 ppm (0.5-4.0 mg/m<sup>3</sup>) [104]

0.21 ppm (0.5 mg/m<sup>3</sup>) [107]

0.2-15 ppm (0.5-34.5 mg/m<sup>3</sup>) [32]

Carcinogenicity: possible [51]; inadequate evidence [55]  
very weak or noncarcinogenic [29]

Mutagenicity: unknown

**Exposure:**

**External:**

Non-lethal: 0.5 ppm (1.15 mg/m<sup>3</sup>) for 12 min -- eye irritation [51]  
 0.8-1.2 ppm (1.8-2.75 mg/m<sup>3</sup>) for 5-10 min -- just tolerable  
 to extremely irritating [104]  
 1.8 ppm (4mg/m<sup>3</sup>) for 4 min -- tolerable [104]  
 4 ppm for 5 min -- severely irritating to eyes [104]  
 Lethal: 250 mg/kg body wt -- injected intradermally [51]

**Oral:**

Non-lethal: unknown  
 Lethal: <50 mg/kg body wt [107]

**Inhalation:**

Short-term Inhalation Limits: 0.5 ppm (1.15 mg/m<sup>3</sup>) for 5 min [107]  
 0.2 ppm (0.5 mg/m<sup>3</sup>) for 60 min [107]  
 Non-lethal: 1 ppm (2.3 mg/m<sup>3</sup>) -- irritation [51]  
 0.3 ppm for 2 hr -- severe pulmonary effects in child [51]  
 Lethal: 150 ppm (345 mg/m<sup>3</sup>) for 10 min [104],[51],[55]  
 5.5 ppm [55]

## 100 - Acrylonitrile

Acrylonitrile

 $C_3H_3N$ 

CAS RN: 107-13-1

Syn: Acrylonitrile \* 2-Propenenitrile \* Acritet \* Acrylon \* Acrylonitrile, inhibited \* Acrylonitrile monomer \* AN \* Carbacryl \* Cyanoethylene \* ENT 54 \* Fumigrain \* Fumugrain \* Miller's Fumigrain \* Nitrile propenoic acid \* Propenenitrile \* RCRA Waste Number U009 \* TL 314 \* UN 1093 (DOT) \* VCN \* Ventox \* Vinyl cyanide \*

Molecular formula:  $CH_2=CHCN$ 

Unsaturated Nitrile

## Physical properties:

Relative molecular mass:	53.0635	
Specific gravity:	0.8075	[107]
	0.8060	[49], [105], [10], [51], [106]
Boiling point:	77.5°-77.9°C	[105]
	77.4°C	[10], [104], [107]
	77.3°C	[49], [51]
	77.3°-77.4°C	[22]
Melting point:	-82.0°C	[51]
	-83.0°C	[51], [104]
	-83.5°C	[105], [106]
	-83.55°C (fp)	[49]
	-83.6°C (fp)	[107]
	-83.7°C	[10]
	-83.°- -84°C	[22]
Refractive index:	1.3911	[10], [105], [106]
	1.3888 @ 25°C	[49]
Vapor pressure:	5.333 kPa @ 3.8°C (40mm)	[105]
	11.0 @ 20°C (83mm)	[49]
	13.332 @ 22.8°C (100mm)	[105], [51]
	13.332 @ 23°C (100mm)	[104]
	14.37 @ 25°C (108mm)	[23]
	18.265 @ 30°C (137mm)	[104]
Vapor density:	1.83	[104], [51]
	1.8	[107]
Evaporation rate:	unknown	
Relative dielectric permittivity:	33.0 @ 20°C	[49], [10]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	263.°C	[107]
	246.°C	[49]
Critical pressure:	4.6 MPa	[107]
	3.54	[49]
Dynamic viscosity:	0.35 mPa-s @ 20°C	[10]
Kinematic viscosity:	0.43 $\mu m^2/s$ @ 20°C	
Surface tension:	29.58 mN/m @ 0°C	[10]
([10] values are calculated)		
	28.40 @ 10°C	[10]
	27.53 @ 17.8°C	[49]
	27.22 @ 20°C	[10]
	27.3 @ 24°C	[49]
	26.05 @ 30°C	[10]
	24.87 @ 40°C	[10]

Contact angle:	unknown	
Thermal expansion coefficient:	0.00146 K <sup>-1</sup> @ 55°C	[49]
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	12.9x10 <sup>-30</sup> C-m in benzene	[49],[10],[105]
Ionization potential:	10.91 eV (PI)	[105]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	6.230 kJ/mol	[49]
	6.229	[10]
Heat of vaporization:	33.249 kJ/mol	[105]
	32.68	[107]
	32.66	[10]
	32.55	[49]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.1110 kJ/(mol-K) (liq)	[105]
	0.10880 (liq)	[49]
	0.0638 (gas)	[10]
	0.0624 (gas)	[105]
Heat of combustion:	-1756.40 kJ/mol @ 25°C (liq)	[49]
Heat of formation:	151.1 kJ/mol @ 25°C (liq)	[10]
	147.11 (liq)	[49]
	185.1 (gas)	[10]
	179.70 (gas)	[49]
Gibbs (free) energy:	195.44 kJ/mol @ 25°C (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	0.92	[104]
	0.25	[23],[31]
	0.14	[8]
	-0.92	[21]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	0.0111 kPa-m <sup>3</sup> /mol @ 25°C	[41]
Hydrolysis half-life =	NA	[8]

**Electrochemical data:** Meites and Zuman (1977), Meites et al. (1977a), Meites et al. (1977b), Horner (1983), Meites et al. (1983)

**Clay-organic interaction data:** Blumstein et al. (1974), Greenland (1972), Mortensen (1959, 1962), Yamanaka et al. (1971).

**Solubility:** Soluble in water, acetone, benzene, and all common organic solvents. Very soluble in hot water. Miscible with ethanol, ether.

[10],[105]

7.35 wt% in water @ 20°C	[49]
7.5 vol% in water @ 25°C	[23]

## 102 - Acrylonitrile

**Form:** Colorless to light yellow liquid. Mild pungent odor resembling that of peach seed kernels, onion, or garlic. 35-45 ppm methylhydroquinone is added as an inhibitor to polymerization. Technical grades are 98-100% pure. [107]

**Use:** Major use is in production of acrylic and modacrylic fibers by copolymerization with methylacrylate, methylmethacrylate, vinyl acetate, vinyl chloride, or vinylidenechloride. Manufacture of synthetic fibers, acrylostryrene plastics, acrylonitrile-butadiene-styrene (ABS) plastics, styrene-acrylonitrile (SAN) resins, nitrile rubbers, chemicals, adhesives; pesticide; cyanoethylation of cotton; synthetic soil blocks (acrylonitrile polymerization in wood pulp); monomer for a semiconductive polymer that can be used like inorganic oxide catalysts in dehydrogenation of tert-butyl alcohol to isobutylene and water; bottles for soft drinks. Carbacryl contains equal portions of acrylonitrile and  $\text{CCl}_4$ . Ventox = acritet = 34% acrylonitrile and 60%  $\text{CCl}_4$ . About 1.5 billion pounds produced annually in the U.S. [56],[104],[5],[22]

**Fire and explosion hazard:** High.

Flash point: (CC)  $-1.11^\circ\text{C}$  [107],[51]

(OC)  $-0.55^\circ\text{C}$  [107]

(OC)  $0^\circ\text{C}$  [49]

uel: 17% [51],[107]

lel: 3.1% [51]

3.05% [107]

Autoign. temp.:  $481^\circ\text{C}$  [51],[107]

Extremely flammable and explosive liquid and poison. Dangerous fire hazard when exposed to heat, flame, or oxidizers. Moderate explosion hazard when exposed to flame. May polymerize and explode. Emits toxic hydrogen cyanide gas and nitrogen oxides when heated to decomposition. Can react vigorously with oxidizing materials. Flashback along vapor trail may occur. Fight fire with  $\text{CO}_2$ , dry chemical powder, alcohol or polymer foam. Water or foam may cause frothing. Cool exposed containers with water. [51],[107],[56]

**Incompatibility:** Light ; heat; strong oxidizers (especially bromine); strong acids; strong alkalis; amines;  $\text{AgNO}_3$ ; ammonia; benzyltrimethyl ammonium hydroxide;  $\text{Br}_2$ ; 1,2,3,4-tetrahydrocarbazole. High concentrations attack aluminum. Attacks copper and copper alloys. [51],[107],[56]

**Handling:** Avoid heat, flame, sources of ignition, air, and visible light. Prevent inhalation of mist or vapor (appropriate respirator or self-contained breathing apparatus required). Wear protective clothing to prevent any skin or eye contact (neoprene, butyl, CPE, or nitrile suit and gloves; splash-proof chemical goggles). Do not use leather as protective clothing. Penetrates leather so contaminated boots and gloves should be destroyed. Readily absorbed through skin. Facilities for eye wash and quick body drenching should be available. Keep container tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet. Store in secure poison area away from light. [107],[53],[55]

**Health effects:** Acrylonitrile closely resemble hydrogen cyanide in its toxic action. Routes of entry are absorption through skin, ingestion, inhalation, and eye and skin contact. Points of attack include the cardiovascular system, liver, kidneys, central nervous system, and skin. It is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Exposure to low concentrations may result in flushing of the face and salivation. Further exposure results in eye and nose irritation, photophobia, and deepened respiration. If exposure continues then shallow respiration, nausea, vomiting, weakness, an oppressive feeling of the chest, headache, and diarrhea may result. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. It is a suspected human carcinogen. [1],[56],[55]

**Toxicity:** High.

TWA: 2 ppm (4.5 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: 4 ppm (9 mg/m<sup>3</sup>) [51]

IDLH: 4 ppm (9 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 21.4 ppm -- sense of smell fatigues rapidly [107]

1.7-23 ppm (3.72-51.0 mg/m<sup>3</sup>) -- recognition [104]

Carcinogenicity: suspected human carcinogen [1],[51]

limited evidence [55]

Mutagenicity: equivocal tumorigenic agent by RTECS criteria [55]

**Exposure:**

**External:**

Non-lethal: 500 mg -- non-standard skin exposure [55]

Lethal: 2015 mg/kg -- on skin of child [55]

**Oral:**

Non-lethal: unknown

Lethal: unknown

**Inhalation:**

Short-term Inhalation Limits: 40 ppm (87 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: 50 ppm (109 mg/m<sup>3</sup>) for 30 min -- blood effects [51]

16 ppm for 20 min -- systemic irritant, CNS effects [51]

Lethal: 46 ppm (1 g/m<sup>3</sup>) per hour -- adult male [55]

## 104 - Aldrin

Aldrin

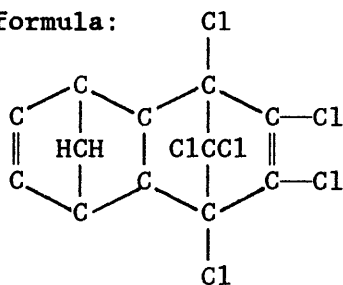
 $C_{12}H_8Cl_6$ 

CAS RN: 309-00-2

Syn: Aldrin \* 1,4:5,8-dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, (1 $\alpha$ ,4 $\alpha$ ,4a $\beta$ ,5 $\alpha$ ,8 $\alpha$ ,8a $\beta$ )- \* Aldocit \* Aldrec \* Aldrex \* Aldrex 30 \* Aldrite \* Aldrosol \* Compound 118 \* Drinox \* ENT 15949 \* 1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, *endo,exo*- \* Hexachlorohexahydro-*endo,exo*-dimethanonaphthalene \* 1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-1,4:5,8-dimethanonaphthalene \* 1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-*exo*-1,4-*endo*-5,8-dimethanonaphthalene \* 1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-1,4-*endo-exo*-5,8-dimethanonaphthalene \* HHDN \* Kortofin \* NA 2761 \* NA 2762 \* NCI-C00044 \* Octalene \* RCRA Waste Number P004 \* SD 2794 \* Seedrin \* Seedrin liquid \* Tatuzinno \* Tipula \*

Molecular formula:  $C_{12}H_8Cl_6$  Polychlorinated Cyclic Aromatic Hydrocarbon

Structural formula:



Physical properties:

Relative molecular mass:	364.914	
Specific gravity:	1.6	[107]
	1.7	[41]
Boiling point:	145.°C at 0.267 kPa	[41]
Melting point:	104.°-105.5°C	[104], [22]
	104.°-105°C	[51]
	104.°C	[105], [107], [56], [106]
	49.°-60°C (technical grades)	[56], [104]
Refractive index:	unknown	
Vapor pressure:	3.07x10 <sup>-6</sup> kPa @ 20°C (2.3x10 <sup>-5</sup> mm)	[104]
	8.0x10 <sup>-7</sup> @ 20°C (6x10 <sup>-6</sup> mm)	[41]
	9.9x10 <sup>-6</sup> @ 20°C (7.5x10 <sup>-5</sup> mm)	[41]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	



Solution diffusivity:	unknown
Electric dipole moment:	unknown
Ionization potential:	unknown
Magnetic volume susceptibility:	unknown
Speed of sound:	unknown
Heat of melting:	unknown
Heat of vaporization:	unknown
Heat of sublimation:	unknown
Heat capacity @ 25°C:	unknown
Heat of combustion:	unknown
Heat of formation:	unknown
Gibbs (free) energy:	unknown

Analytical chemistry:	pP <sub>oct</sub> =	5.66	[27]
		5.52	[41]
		5.30	[31]
		3.01	[21]
	pK <sub>s</sub> =	NA	
	pK <sub>a</sub> =	NA	[31]
	pK <sub>BH</sub> =	NA	
Henry's law constant =		0.0503 kPa·m <sup>3</sup> /mol	[41]
		0.00014	[41]
Hydrolysis half-life =		>1.3x10 <sup>8</sup> sec	[8]

**Electrochemical data:** Unknown

Clay-organic interaction data: Kenega and Goring (1980).

**Solubility:** Almost insoluble in water. Soluble in ethanol, ether, acetone, benzene, aromatics, esters, ketones, paraffins, halogenated solvents, most organic solvents. [51]

0.000001 wt% in water [104]

Form: Colorless, crystalline solid. Technical grade is a tan to dark brown solid or solution. Mild, chemical odor. Commercial grades range in purity from 20-95% with 5-80% inert ingredients. Readily oxidizes to Dieldrin. [51],[107],[56]

**Use:** Pesticide; insecticide; fumigant. Use was restricted by U.S. government in 1974. [56],[104]

**Fire and explosion hazard:** Very low.

Flash point: NA

ue1: NA

1e1: NA

Autoign. temp.: NA

Nonflammable solid. Emits toxic fumes of  $\text{Cl}^-$  and hydrochloric acid when heated to decomposition. Fight fires involving Aldrin solution in hydrocarbon solvents with water spray, dry chemical powder, alcohol or polymer foam,  $\text{CO}_2$ . [51],[107]

**Incompatibility:** No reaction with most common materials. [107],[56]

## 106 - Aldrin

**Handling:** Wear protective clothing to prevent any possibility of skin or eye contact (synthetic rubber gloves and suit, splash-proof chemical goggles). Appropriate respirator or self-contained breathing apparatus required. Facilities for eye wash and quick body drenching should be available. Keep container tightly closed. Store in secure poison area. [107],[56]

**Health effects:** Aldrin is a poison. Routes of entry are inhalation, skin absorption, ingestion, and eye and skin contact. Points of attack include the central nervous system, liver, kidneys, and skin. It is irritating to the skin, eyes and respiratory system. Symptoms of exposure are irritability, headache, dizziness, hyperexcitability, epileptiform convulsions, tremors, nausea and depression in from 1 to 5 hrs. Continued exposure can cause reversible kidney and liver damage. [51],[107],[56]

**Toxicity:** High.

TWA: 0.017 ppm (0.25 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 6.7 ppm (100 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 0.017 mg/kg in water [104]

Carcinogenicity: experimentally positive in some animals. [51]

Mutagenicity: experimentally positive in some animals. [51]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: 14 mg/kg body wt -- CNS effects [51]

1 g -- symptoms [107]

Lethal: 1.25 mg/kg body wt -- death of a child [51]

25 mg in children [107]

Inhalation:

Short-term Inhalation Limits: 0.07 ppm (1 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: unknown

Lethal: unknown

## Ammonia



CAS RN: 7664-41-7

Syn: Ammonia \* Am-fol \* Ammonia gas \* Anhydrous ammonia \* Liquid ammonia \* Nitro-Sil \* R 717 \* Spirit of Hartshorn \* UN 1005 (DOT) \* UN 2073 (DOT) \*

Molecular formula: NH<sub>3</sub>

Inorganic Nitrogen Compound

## Physical properties:

Relative molecular mass:	17.0305	
Specific gravity:	0.7714 kg/m <sup>3</sup> @ 0°C (gas)	[48]
	0.771 g/L @ 0°C (gas)	[51], [105]
	0.7708 g/L @ 0°C (gas)	[10]
	0.7188 g/L @ 20°C (gas)	[10]
	0.77 @ 0°C (liq)	[22]
	0.6819 @ -33.5°C (liq)	[22]
	0.682 @ -33.4°C (liq)	[107]
	0.6818 @ -33.35°C (liq)	[10]
	0.67 @ -33.4°C	[32]
	0.817 g/L @ -79°C	[51], [104]
Boiling point:	-33.35°C	[51], [10], [105], [48], [7]
	-33.4°C	[47], [107], [104], [32]
	-33.42°C	[10]
	-35.5°C	[22]
Melting point:	-77.70°C	[47], [51], [10], [105], [107], [104]
	-77.75°C	[10]
	-77.9°C	[48]
Refractive index:	1.0003501 (gas)	[10]
	1.325 @ 16°C (liq)	[10]
	1.325 @ 16.5°C (liq)	[105]
	0.817 @ -79°C (liq)	[105]
Vapor pressure:	290.83 kPa @ -10°C (2181.4mm)	[10]
	429.41 @ 0°C (3220.9mm)	[10]
	476.3 @ 4.7°C (3572mm)	[105]
	614.89 @ 10°C (4612.1mm)	[10]
	857.06 @ 20°C (6428.5mm)	[10]
	861.28 @ 20°C (6460mm)	[22]
	881.53 @ 20°C (6612mm)	[104]
	1013.25 @ 25.7°C (7600mm)	[51], [105]
	1166.5 @ 30°C (8749.1mm)	[10]
Vapor density:	0.6	[51], [107], [104]
	0.5962	[10]
Evaporation rate:	NA	
Relative dielectric permittivity:	25.0 @ -77.7°C (liq)	[20]
	22.4 @ -33.4°C (liq)	[20], [10]
	22.0 @ -33°C (liq)	[10], [11]
	15.0 @ -24°C (liq)	[11]
	1.0072 @ 0°C (gas) <3 MHz	[10], [105]
	1.007 @ 0°C (gas)	[11]
	18.9 @ 5°C	[20]
	17.8 @ 15°C	[20]
	16.9 @ 25°C	[20]
	16.3 @ 35°C	[20]
Loss tangent:	unknown	
Relaxation time:	unknown	

## 108 - Ammonia

Thermal conductivity:	1.60 W/(m-K) @ -57.6°C (liq)	[10]
	2.150 @ 0°C (liq)	[10]
	2.97 @ 100°C (liq)	[10]
	0.02024 @ -17.8°C (gas)	[10]
	0.02232 @ 4.4°C (gas)	[10]
	0.02336 @ 15.6°C (gas)	[10]
	0.02457 @ 26.7°C (gas)	[10]
Electrical resistivity:	0.0769 MOhm-m @ -79°C	[10]
Critical temperature:	132.9°C	[10]
	132.5°C	[105]
	132.44°C	[7]
	132.4°C	[10], [48]
Critical pressure:	11.44 MPa	[48]
	11.40	[105]
	11.38	[10]
	11.30	[7]
	11.28	[10]
	11.27	[107]
Dynamic viscosity:	0.254 mPa-s @ -33.5°C	[10]
Kinematic viscosity:	0.372 $\mu\text{m}^2/\text{s}$ @ -33.5°C	
Surface tension:	37.91 mN/m @ -50°C (liq)	[10]
	35.38 @ -40°C (liq)	[10]
	23.4 @ 11.1°C	[20], [105]
	18.1 @ 34.1°C	[20], [105]
Contact angle:	NA	
Thermal expansion coefficient:	NA	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	2.0 nm <sup>2</sup> /s in water	[47]
Electric dipole moment:	4.90x10 <sup>-30</sup> C-m (gas)	[10], [105]
Ionization potential:	10.2 eV (S,PI,PE)	[105]
Magnetic volume susceptibility:	-56.5x10 <sup>-6</sup> SI units @°C	[105]
Speed of sound:	415.0 m/s @ 0°C	[105]
Heat of melting:	5.656 kJ/mol	[10]
Heat of vaporization:	23.36 kJ/mol (gas)	[10], [107]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.0351 kJ/(mol-K) (gas)	[10], [105]
Heat of combustion:	-316.6 kJ/mol @ 25°C (gas)	[107]
Heat of formation:	-46.14 kJ/mol @ 25°C (gas)	[10], [20], [105]
	-46.22 (gas)	[7]
Gibbs (free) energy:	-16.50 kJ/mol @ 25°C (gas)	[10], [105]
Analytical chemistry:	pP <sub>oct</sub> = unknown	
	pK <sub>s</sub> = 33.0 @ -50°C	[10]
	pK <sub>a</sub> = NA	
	pK <sub>BH</sub> = 4.67 @ 18°C	[11]
	pK <sub>BH</sub> = 4.767 @ 20°C in water	[105]
	Henry's law constant = unknown	
	Hydrolysis half-life = unknown	

Electrochemical data: Reed and Wightman (1984)

Clay-organic interaction data: Mortland et al. (1963), Russell (1965)

**Solubility:** Soluble in ethanol, other organic solvents. Very soluble in cool water. [10],[105]

89.5 wt% in water @ 0°C	[104]
89.9 wt% in cold water	[105],[10]
53.1 wt% in water @ 20°C	[104]
51. wt% in water @ 20°C	[32]
44.0 wt% in water @ 28°C	[104]
7.4 wt% in water @ 100°C	[105]
13.2 wt% in ethanol @ 20°C	[10],[105]
20.95 wt% in ethanol @ 0°C	[7]
29.3 wt% in methanol @ 0°C	[7]

**Form:** Colorless gas. Liquified by compression for shipping. Extremely pungent, suffocating odor. [51],[107]

**Use:** As a nitrogen source for many nitrogen-containing compounds; refrigerant; petroleum refining and chemical industries; in the production of many drugs and pesticides, ammonium sulfate and ammonium nitrate for fertilizers; manufacture of nitric acid, soda, synthetic urea, synthetic fibers (cupramonium rayon and nylon), dyes, and plastics; copper, nickel, and molybdenum ore extraction and purification; in dilute forms as household cleansing agent; developing diazo film; rocket fuel; yeast nutrient; sulfite cooking liquors; solvent in manufacture of textiles, leather, and pulp and paper processing. Ammonia is a combustion by-product of coal, fuel oil, natural gas, butane, propane, wood, forest fires. Third highest volume chemical produced in U.S. in 1975. [107],[56],[104],[22],[32]

**Fire and explosion hazard:** Low

Flash point: unknown

UEL: 25% [51],[105]

27% [10],[107]

LEL: 16% [51],[105]

15.5% [10]

15% [107]

Autoign. temp.: 651.1°C [51],[105],[107],[32]

Nonflammable gas. Low fire hazard because it is difficult to light when exposed to heat or flame. Requires high concentrations before catching fire. Moderate explosion hazard when exposed to flame or in a fire.  $\text{NH}_3$  + air can detonate in a fire. Emits highly toxic fumes of  $\text{NH}_3$  and  $\text{NO}_x$  when heated to decomposition. Fight fire by stopping flow of gas or liquid if possible. Cool exposed containers and protect persons effecting supply shutoff with water. Let fire burn. Do not extinguish burning gas if flow cannot be shut off immediately. [51],[107],[55]

**Incompatibility:** Strong oxidizers; acetaldehyde; acrolein; boron;  $\text{HClO}_3$ ; chlorites; chlorosilane; Cu; (ethylene dichloride + liquid ammonia); ethylene oxide; galvanized surfaces; hexachloromelamine; (hydrazine + alkali metals);  $\text{HBr}$ ;  $\text{HOCl}$ ; hypochlorite bleaches;  $\text{N}_2\text{O}_4$ ;  $\text{NCl}_3$ ;  $\text{NF}_3$ ;  $\text{OF}_2$ ;  $\text{P}_2\text{O}_5$ ;  $\text{P}_2\text{O}_3$ ; picric acid; ( $\text{K} + \text{AsH}_3$ ); ( $\text{K} + \text{PH}_3$ ); ( $\text{K} + \text{NaNO}_2$ ); potassium ferricyanide; potassium mercuric cyanide;  $\text{AgCl}$ ; ( $\text{Na} + \text{CO}$ ); Sb; S;  $\text{SbCl}_2$ ; tellurium hydropentachloride; trichloromelamine; boron halides; ethylene oxide;  $\text{NO}_2\text{Cl}$ ; gold(III)chloride;  $\text{CrO}_3$ ; ammonium peroxy disulfate; ( $\text{O}_2 + \text{Pt}$ );  $\text{AgNO}_3$ ;  $\text{Ag}_2\text{O}$ ;  $\text{SbH}_3$ ;  $\text{SOCl}_2$ . WARNING: ammonia reacts violently, or

## 110 - Ammonia

produces explosive products, with all four halogens and with some of the interhalogens such as bromine pentafluoride, chlorine trifluoride. It reacts with some heavy metals and their salts (i.e. mercury, silver, gold) to produce materials of a sometimes unknown composition that are shock-sensitive and may explode when dry. At ambient temperature, ammonia gas reacts exothermically with calcium, but if warmed the latter becomes incandescent. Reaction of ammonia with 2-nitro, 4-nitro or 2,4-dinitro chlorobenzene may result in violent runaway reactions producing high internal pressures causing rupture of equipment. Reaction with tellurium tetrabromide or tetrachloride forms tellurium nitride which explodes on heating. Thiocarbonyl azide rapidly absorbed ammonia gas and then exploded. A heated mixture of stibine and ammonia explodes.

Tetramethylammonium amide decomposes explosively at ambient temperature in the presence of ammonia. Thiocarbonyl azide thiocyanate reacts explosively with ammonia gas. Ammonia gas reacts violently when mixed with: magnesium perchlorate, potassium chlorate, nitryl chloride, dichlorine oxide, chromyl chloride, chromium trioxide, trioxxygen difluoride, nitric acid, hydrogen peroxide, ammonium persulfate, nitric oxide, nitrogen dioxide, pentaborane, boron trihalides, chlorine azide or chloroformamidinium nitrate.

[51],[107],[56],[32],[55]

**Handling:** Avoid sparks near air and gas mixture within explosion limit range. Wear protective clothing to prevent skin contact with the liquid or solutions >10 wt% ammonia (butyl, natural rubber, neoprene, nitrile or PVC apron, boots and gloves; splash-proof safety goggles). Gas-tight chemical goggles and appropriate respirator or self-contained breathing apparatus required to prevent eye contact and inhalation of the gas. Facilities for eye wash and quick body drenching should be available. Store at ambient temperature for pressurized ammonia; low temperature for ammonia at atmospheric pressure. Withdraw gas from cylinders in well-ventilated area or fume hood. Cylinder temperature should not exceed 52°C (125°F). Use with equipment rated for cylinder pressure, and of compatible materials of construction. Close valve when not in use and when empty. Make sure cylinder is properly secured when in use or stored.

[107],[56],[53],[32],[55]

**Health effects:** Ammonia is considered a poison and is corrosive. Routes of entry are inhalation of gas, ingestion, skin absorption, and eye and skin contact. Points of attack include lungs, respiratory system, and eyes. Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. Symptoms of exposure are tearing and burning of the eyes, runny nose, conjunctivitis (swelling of the eyelids), nose and throat irritation, coughing, chest pain, dyspnea, and vomiting. Vapors cannot be tolerated even at low concentrations. Contact of liquid or solid with skin causes first degree burns on short exposure and second degree burns on longer exposure. Corneal ulcers have been reported after splashing ammonia water in the eyes. Ammonia is a common air contaminant.

[51],[56],[6],[55]

**Toxicity: Moderate**

TWA: 25 ppm (18 mg/m<sup>3</sup>) [1]  
STEL: 35 ppm (27 mg/m<sup>3</sup>) [1]  
CL: 50 ppm (35 mg/m<sup>3</sup>) [51],[56]  
IDLH: 500 ppm (350 mg/m<sup>3</sup>) [107],[56]  
Peak: unknown  
Odor threshold: 46.8 ppm (33 mg/m<sup>3</sup>) [107]  
0.5-70 ppm (0.4-50 mg/m<sup>3</sup>) [104]  
20 ppm (14 mg/m<sup>3</sup>) [7]  
1-5 ppm (0.7-3.5 mg/m<sup>3</sup>) [32]  
Carcinogenicity: unknown  
Mutagenicity: unknown

**Exposure:****External:**

Non-lethal: 140 ppm -- eye and respiratory tract irritation [51],[32]  
100 ppm -- eye and nasal passage irritation [7]  
400-700 ppm (280-490 mg/m<sup>3</sup>) -- severe eye, nose and throat  
irritation which may result in permanent injury if  
prompt measures are not taken [107]  
10000 ppm -- mildly irritating to moist skin [32]  
30000 ppm (21000 mg/m<sup>3</sup>) -- skin burns and vesiculation [32]

Lethal: unknown

**Oral:**

Non-lethal: unknown  
Lethal: 132 mg/kg body wt. -- death of an adult male [51]

**Inhalation:**

Short-term Inhalation Limits: 50 ppm (35 mg/m<sup>3</sup>) for 5 min [107]  
Non-lethal: 20-32 ppm -- irritation for some persons [51],[32]  
>25 ppm (18 mg/m<sup>3</sup>) -- unsatisfactory [107]  
134 ppm -- irritation of eyes, nose and throat [32]  
2500-6500 ppm (1.7-4.5 g/m<sup>3</sup>) -- dyspnea, bronchospasm,  
chest pain, pulmonary edema which may be fatal [32]  
Lethal: 30000 ppm (21 g/m<sup>3</sup>) for 5 min -- death of an adult human [51]  
5000-10000 ppm (3.5-7 g/m<sup>3</sup>) for a few min [6],[7]  
1700 ppm (1180 mg/m<sup>3</sup>) for 30 min [7]

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Aniline

 $C_6H_7N$ 

CAS RN: 62-53-3

Syn: Aniline \* Benzenamine \* Aminobenzene \* Aminophen \* Aniline oil \*  
 Arylamine \* Anyvim \* Benzene, amino \* Benzidam \* Blue oil \* C.I. 76000 \*  
 C.I. oxidation base 1 \* Cyanol Krystallin \* Kyanol \* NCI-C03736 \*  
 Phenylamine \* RCRA Waste Number U012 \* UN 1547 (DOT) \*

Molecular formula:  $C_6H_5-NH_2$ 

Primary Aromatic Amine

## Physical properties:

Relative molecular mass:	93.1283	
Specific gravity:	1.0235	[22]
	1.02173	[105], [49]
	1.0217	[10], [106]
	1.022	[107], [10], [48], [32]
	1.02	[51], [104]
Boiling point:	184.4°C	[49], [10], [51], [22]
	184.2°C	[107]
	184.0°C	[105], [56], [104], [48], [32]
Melting point:	-6.3°C	[105], [106]
	-6.2°C	[51], [48], [22], [32]
	-6.1°C	[107]
	-6.0°C	[104]
	-5.98°C	[10], [49]
Refractive index:	1.5863	[105], [22], [106]
	1.58628	[49]
	1.5855	[10]
Vapor pressure:	0.04 kPa @ 20°C (0.3mm)	[104]
	0.08 @ 20°C (0.6mm)	[32]
	0.065 @ 25°C (0.489mm)	[23]
	0.0895 @ 25°C (0.671mm)	[49]
	0.13 @ 34.8°C (1mm)	[105], [51]
	0.13 @ 35°C (1mm)	[104]
Vapor density:	3.22	[51], [104], [32]
Evaporation rate:	<1.0	[32]
Relative dielectric permittivity:	7.04 @ 17°C (3 MHz)	[2]
	7.20 @ 20°C (3 MHz)	[2]
	7.06 @ 20°C (1.8MHz)	[2]
	6.89 @ 20°C	[10], [105], [11]
	6.77 @ 25°C	[2]
	7.06 @ 25°C (1.8 MHz)	[2]
	6.71 @ 30°C	[49]
	5.93 @ 70°C	[105], [11]
	5.932 @ 70°C (180 MHz)	[2]
	4.54 @ 184.6°C	[105]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.1708 W/(m-K) @ 12°C	[10]
	0.172 @ 0°-50°C	[48]
	0.1774 @ 16.5°C	[105]
Electrical resistivity:	0.417 MOhm-m @ 25°C	[10], [49], [11]
	0.122 @ 35°C	[11]
Critical temperature:	426.0°C	[49], [10]
	425.6°C	[105], [107]



Critical pressure:	52.5 MPa	[105], [107]	
	52.39	[49]	
	5.31	[10]	
Dynamic viscosity:	13.8 mPa-s @ -6°C	[105]	
	10.2 @ 0°C	[105], [48]	
	8.06 @ 5°C	[105], [48]	
	6.50 @ 10°C	[105], [48]	
	5.31 @ 15°C	[105], [48]	
	4.43 @ 20°C	[48]	
	4.40 @ 20°C	[10], [105]	
	3.71 @ 25°C	[105], [48]	
	3.23 @ 30°C	[48]	
	3.16 @ 30°C	[105]	
	2.79 @ 35°C	[48]	
	2.71 @ 35°C	[105]	
	2.37 @ 40°C	[105], [48]	
	1.85 @ 50°C	[105]	
	1.51 @ 60°C	[105]	
	1.27 @ 70°C	[105]	
	1.09 @ 80°C	[105]	
	0.935 @ 90°C	[105]	
	0.825 @ 100°C	[105]	
Kinematic viscosity:	13.5 $\mu\text{m}^2/\text{s}$ @ -6°C		
	9.98 @ 0°C		
	7.89 @ 5°C		
	6.36 @ 10°C		
	5.20 @ 15°C		
	4.33 @ 20°C		
	4.31 @ 20°C		
	3.63 @ 25°C		
	3.16 @ 30°C		
	3.09 @ 30°C		
	2.73 @ 35°C		
	2.65 @ 35°C		
	2.32 @ 40°C		
	1.81 @ 50°C		
	1.48 @ 60°C		
	1.24 @ 70°C		
	1.07 @ 80°C		
	0.915 @ 90°C		
	0.807 @ 100°C		
Surface tension:	44.1 mN/m @ 10°C (air)	[105]	
	43.38 @ 19°C	[49]	
	42.9 @ 20°C (vapor)	[105]	
	45.5 @ 20°C	[107]	
	42.79 @ 25°C	[49]	
	42.01 @ 32°C	[49]	
	39.4 @ 50°C (air)	[105]	
Contact angle: [18]			
	sessile	advancing	receding
quartz	41	38	24
calcite	46	48	30
biotite	38	43	24
Ca-mont.	0	0	0

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Thermal expansion coefficient:	0.00085 K <sup>-1</sup> @ 20°C	[48]
Compressibility:	0.408 nPa <sup>-1</sup> @ 0°C	[105]
	0.430 10°C	[105]
	0.453 20°C	[105]
	0.467 25°C	[105]
	0.504 40°C	[105]
	0.522 45°C	[105]
	0.533 50°C	[105]
	0.564 60°C	[105]
	0.584 65°C	[105]
	0.597 70°C	[105]
	0.632 80°C	[105]
	0.656 85°C	[105]
	0.670 90°C	[105]
Vapor diffusivity:	6.1 μm <sup>2</sup> /s @ 0°C in air	[47]
	7.5 @ 30°C in air	[47]
Solution diffusivity:	unknown	
Electric dipole moment:	5.104x10 <sup>-30</sup> C-m	[105], [10]
	5.04x10 <sup>-30</sup>	[49]
Ionization potential:	7.7 eV (PI)	[105]
Magnetic volume susceptibility:	-8.68x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	10.55 kJ/mol	[105], [10]
Heat of vaporization:	47.343 kJ/mol	[105]
	44.560	[10]
	44.530	[49]
	42.9	[107]
Heat of sublimation:	55.789 kJ/mol	[10]
Heat capacity @ 25°C:	0.1934 kJ/ (mol-K) (liq)	[105]
	0.1922 (liq)	[10]
	0.19101 (liq)	[49]
	0.1085 (gas)	[10]
Heat of combustion:	-3398.4 kJ/mol @ 20°C (liq)	[105]
	-3391.1 @ 25°C (liq)	[49]
Heat of formation:	31.61 kJ/mol @ 25°C (liq)	[10]
	31.25 (liq)	[49]
	86.92 (gas)	[10]
Gibbs (free) energy:	149.2 kJ/mol @ 25°C (liq)	[10]
	166.8 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	0.98	[104], [21], [27]
	0.90	[104], [23], [21]
	0.89	[21]
	0.85	[21]
pK <sub>s</sub> =	unknown	
pK <sub>a</sub> =	4.596	[23]
	4.63 @ 25°C	[105]
pK <sub>BH</sub> =	9.42	[11]
	4.60 @ 25°C in water	[49]
	4.606 @ 25°C in aqueous HCl	[49]
Henry's law constant =	unknown	
Hydrolysis half-life =	unknown	

**Electrochemical data:** Meites and Zuman (1977), Meites et al. (1977a), Meites et al. (1982), Lines (1983)

**Clay-organic interaction data:** Aniline increases hydraulic conductivity of clay soils (Anderson and Brown, 1981; Anderson et al., 1981; Briggs, 1981; Brown et al., 1984; Evans et al., 1985; Furukawa and Brindley, 1973; Greene-Kelly, 1955; Heller and Yariv, 1969; Pillai et al., 1982; Tennakoon et al., 1974; Yariv et al., 1968, 1969).

**Solubility:** Slightly soluble in water. Soluble in carbon tetrachloride, ligroin. Miscible with hot water, ethanol, ether, acetone, benzene.

[10],[49],[104]

3.4 wt% in water [104]

3.6 wt% in water @ 18°C [10]

3.38 wt% @ 25°C in water [49]

**Form:** Colorless oily liquid. Rapidly becomes pale brown on exposure to air and light. Characteristic, peculiar, aromatic amine-like odor. Commercial grades are 99.5% pure. [56],[51],[22]

**Use:** One of the most important of the organic bases; the parent substance for many dyes and drugs; intermediate in the synthesis of dyestuffs; manufacture of rubber accelerators and antioxidants, pharmaceuticals, marking inks, tetaryl, optical whitening agents, hydroquinone for photographic processing, resins, varnishes, perfumes, shoe polish, many other organic chemicals; herbicides, fungicides, phenolics; petroleum refining. [107],[56],[22],[32]

**Fire and explosion hazard:** Moderate.

Flash point: (CC) 70°C [107],[51],[32]

(CC) 76°C [49]

(OC) 75.5°C [107]

uel: 11% [107]

lel: 1.3% [107],[51],[32]

Autoign. temp.: 615°C [51],[32]

770°C [107],[10]

Flammable liquid. Moderate fire and explosion hazard when exposed to heat or flame. Emits highly toxic fumes of CO, CO<sub>2</sub>, and NO<sub>x</sub> when heated to decomposition. Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical. Stop discharge if possible. Cool exposed containers with water. [51],[107]

**Incompatibility:** Strong acids; strong oxidizers; bases; acetic anhydride; chlorosulfonic acid; hexachloro melamine; HNO<sub>3</sub>; (HNO<sub>3</sub> + N<sub>2</sub>O + H<sub>2</sub>SO<sub>4</sub>); (nitrobenzene + glycerine); oleum; O<sub>3</sub>; (HCHO + HClO<sub>4</sub>); perchromates; performic acid; K<sub>2</sub>O<sub>2</sub>; β-propiolactone; AgClO<sub>4</sub>; Na<sub>2</sub>O<sub>2</sub>; H<sub>2</sub>SO<sub>4</sub>; trichloromelamine; BCl<sub>3</sub>; nitromethane; peroxydisulfuric acid; peroxo mono sulfuric acid; F<sub>2</sub>; FNO<sub>3</sub>; FO<sub>3</sub>Cl; diisopropyl peroxy-dicarbonate; N-haloimides; trichloronitro methane. [51],[56]

**Handling:** Avoid heat, flame, sparks, and other sources of ignition. Wear protective clothing and eye protection to prevent skin contact (butyl, natural rubber, neoprene, or nitrile suit, gloves and boots; splash-proof safety goggles). Contaminated clothing should be removed immediately and not re-worn till the aniline is removed. Appropriate respirator or self-

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contained breathing apparatus required. Use in well-ventilated area (fume hood). Facilities for eye wash and quick body drenching should be available. Keep container tightly closed. Store in cool, dry, well-ventilated, flammable liquid storage area or cabinet. Store in secure poison area. [32],[53]

**Health effects:** Aniline is a poison. Routes of entry are inhalation of vapors, percutaneous absorption of liquid and vapor, ingestion, and skin and eye contact. Points of attack include blood, cardiovascular system, liver, kidneys, eyes, and upper respiratory tract. The most important action on the body is the formation of metahemoglobin, with the resulting anoxemia (lack of oxygen in the blood) and depression of the central nervous system. Onset may be delayed 2 to 4 hours or longer. Local effect of liquid aniline is mild irritation of the eyes and skin with possible corneal damage. Vapor or mist can be irritating to the eyes, mucous membranes and upper respiratory tract. Symptoms following acute exposure are discoloration (cyanosis) of fingertips, cheeks, lips and nose, nausea, vomiting, headache and drowsiness followed by delirium, coma and shock. Chronic exposure may result in loss of appetite, loss of weight, headaches, visual disturbances, irritability, paleness, dizziness, and skin lesions. A common air contaminant. [51],[107],[32]

### **Toxicity:** High.

TWA: 2 ppm (10 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 100 ppm (380 mg/m<sup>3</sup>) [56],[107]

Peak: unknown

Odor threshold: 0.01-0.5 ppm (0.04-2.0 mg/m<sup>3</sup>) -- detection [104]

0.1-1.3 ppm (0.4-5.0 mg/m<sup>3</sup>) -- recognition [104]

0.5 ppm (2.0 mg/m<sup>3</sup>) [107]

0.5-7 ppm (2.0-27 mg/m<sup>3</sup>) [32]

Carcinogenicity: possible [51]

potential human carcinogen (IARC) [32]

Mutagenicity: possible [51],[55]

### **Exposure:**

#### External:

Non-lethal: unknown

Lethal: unknown

#### Oral:

Non-lethal: unknown

Lethal: 150 mg/kg body wt -- death of an adult male [51]

357 mg/kg body wt -- death of an adult human [51]

50-500 mg/kg [107]

#### Inhalation:

Short-term Inhalation Limits: 50 ppm (190 mg/m<sup>3</sup>) for 30 min [107]

5 ppm (20 mg/m<sup>3</sup>) for 8 hr [107]

Non-lethal: 7 ppm (27 mg/m<sup>3</sup>) -- slight symptoms [32]

>10 ppm (38 mg/m<sup>3</sup>) -- unsatisfactory [104]

20 ppm (75 mg/m<sup>3</sup>) -- symptoms of illness may begin [104]

80 ppm (300 mg/m<sup>3</sup>) for 60 min -- severe toxic effects [104]

Lethal: unknown

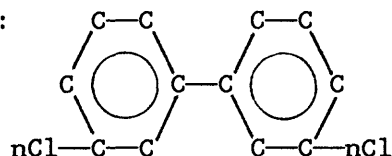
Aroclor 1260 (PCB 1260)

 $(C_{12}H_{10-x})Cl_x$ 

CAS RN: 11096-82-5

Syn: Aroclor 1260 \* Chlorodiphenyl (60% Cl) \* Chlorphen A60 \* Kanechlor \* PCB-1260 \* Phenochlor DP6 \* Polychlorinated biphenyl \* Polychlorobiphenol \* UN 2315 (DOT) \*

Structural formula:



Polychlorinated Hydrocarbon

**Physical properties:**

Relative molecular mass:	varies (375.7 for PCB 1260)	
	321. to 460 (average is 370)	[41]
Specific gravity:	1.4-1.5	[22]
	1.3-1.8	[107]
	1.44 @ 30°C	[51]
Boiling point:	340.-375°C	[51]
Melting point:	31.°C	[41]
Refractive index:	1.627-1.649	[108]
Vapor pressure:	5.40x10 <sup>-6</sup> kPa @ 25°C (4.05x10 <sup>-5</sup> mm)	[8]
	2.7x10 <sup>-8</sup> @ 38°C (2x10 <sup>-7</sup> mm)	[41]
Vapor density:	unknown	
Evaporation rate:	unknown	
Relative dielectric permittivity:	4.3-5.6 @ 25°C	[108]
	3.7-4.9 @ 100°C	[108]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	unknown	
Kinematic viscosity:	unknown	
Surface tension:	unknown	
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	unknown	
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	unknown	
Heat of combustion:	unknown	
Heat of formation:	unknown	
Gibbs (free) energy:	unknown	

Analytical chemistry:  $pP_{oct}$  = 7.14 (est) [8],[31]  
6.91 [41]

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	6.72 for $C_{12}H_4Cl_6$	[21]
	5.58 for $C_{12}H_8Cl_2$	[21]
	4.52-6.70	[27]
$pK_s =$	NA	
$pK_a =$	NA	[31]
$pK_{BH} =$	NA	
Henry's law constant =	0.719 kPa·m <sup>3</sup> /mol	[41]
Hydrolysis half-life =	NA	[8]

**Electrochemical data:** Unknown

**Clay-organic interaction data:** None (Dragun and Helling, 1985)

**Solubility:** The solubility of PCBs in water decreases with increasing chlorination. Soluble in most solvents. [104],[41]

0.04-0.2 ppm in water [104]

**Form:** PCBs are a series of technical mixtures consisting of about 200 isomers and compounds that vary from mobile oily liquids to white crystalline solids and hard noncrystalline resins with typical chlorinated aromatic odors. Technical products vary in composition, in the degree of chlorination, and possibly according to batch. An estimated 40 to 70 different chlorinated biphenyl compounds can be present in each of the higher-chlorinated commercial mixtures. PCBs contain 11 grades of purity (some liquid, some solid) which differ primarily in their chlorine content (20%-60% by weight). 42% chlorodiphenyl is a mobile liquid and 54% chlorodiphenyl is a viscous liquid. The isomer chosen as an example here is Aroclor 1260 which is composed of 12% penta-, 38% hexa-, 41% hepta-, 8% octa-, and 1% nona-chlorobiphenyls. Certain PCB mixtures also contain other classes of chlorinated derivatives including chlorinated naphthalenes and chlorinated dibenzofurans. [56],[107],[51]

**Use:** In electrical capacitors, electrical transformers, vacuum pumps, gas-transmission turbines; in polyester resins to increase strength of fiberglass; varnish formulations to improve water alkali resistance; insulator fluid for electric condensers. Formerly used in the U.S. as hydraulic fluids, plasticizers for polyvinyl chloride, adhesives, fire retardants, dusting agents, pesticide extenders, inks, additive for high-pressure lubricants, cutting oils, in heat transfer systems, carbonless reproducing paper. [108],[56],[41]

**Fire and explosion hazard:** Low.

Flash point: (CC) 195°C [51]

(OC) 195°C [51]

(OC) >141°C [107]

uel: unknown

lel: unknown

Autoign. temp.: unknown

Slightly flammable solid. Dangerous when heated to decomposition; emits highly toxic fumes; fire resistant. Fight fire with water, alcohol or polymer foam, dry chemical, CO<sub>2</sub> [51]

**Incompatibility:** Strong oxidizers. [56]

**Handling:** WARNING: avoid all contact. Keep away from heat and open flame. Do not breathe vapor (appropriate respirator or self-contained breathing apparatus required). Do not get in eyes, on skin, or on clothing (chemical resistant gloves and suit; safety goggles or face shield). Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [56]

**Health effects:** PCBs are highly toxic and suspected carcinogens. Routes of entry are inhalation of dust, mist, or vapor, skin absorption, ingestion, and eye and skin contact. Points of attack include skin, eyes, and liver. The higher the chlorine content of the diphenyl compound the more toxic it is likely to be. Oxides are more toxic than the unoxidized materials. PCBs have two distinct actions on the body, a skin effect and a toxic action on the liver. The skin lesion is known as chloroacne, and consists of small pimples and dark pigmentation of exposed areas, initially. Later, comedones and pustules develop. The signs and symptoms of systematic intoxication are nausea, vomiting, loss of weight, jaundice, edema, and abdominal pain. If the liver damage is severe, the patient may pass into a coma and die. May also cause birth defects. [51],[5],[88]

**Toxicity:** High.

TWA: 1 mg/m<sup>3</sup> (skin) (42% CL) [1]

0.5 mg/m<sup>3</sup> (skin) (54% CL) [1]

STEL: no values set [1]

CL: unknown

IDLH: 5-10 mg/m<sup>3</sup> [107],[56]

Peak: unknown

Odor threshold: practically odorless [107]

Carcinogenicity: suspected human carcinogen [51]

animal positive [56],[51]

Mutagenicity: causes chromosomal abnormalities in rats, birth defects in birds. [107]

**Exposure:** Unknown

**External:**

Non-lethal: unknown

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: unknown

**Inhalation:**

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown

## 120 - Arsenic

Arsenic

As

CAS RN: 7440-38-2

Syn: Arsenic \* Arsenicals \* Arsenic-75 \* Arsenic black \* colloidal arsenic \* Grey arsenic \* Metallic arsenic \* UN 1558 (DOT) \*

Molecular formula: As

Element

## Physical properties:

Relative molecular mass:	74.9216	[105]
Specific gravity:	5.727 @ 14°C (grey)	[105], [47]
	5.727 (25/4)	[108]
	5.724 (black crystals)	[51]
	5.72	[22]
	5.72 (grey)	[10]
	5.6-5.9 (commercial product)	[22]
	4.7 (black amorphous solid)	[51], [10]
	2.026 @ 18°C (yellow)	[105], [10]
	2.0 (yellow)	[47]
Boiling point:	615.0°C sublimes	[47], [108]
	613.0°C sublimes	[10], [105]
	612.0°C sublimes	[51]
Melting point:	817.0°C @ 2837.1 kPa (21280mm)	[10], [105]
	814.0°C @ 3647.7 kPa (27360mm)	[51], [47]
Refractive index:	NA	
Vapor pressure:	0.133 kPa @ 372°C (1mm)	[47], [51]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	10.23 @ 20°C (60 MHz)	[108]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	53.9 W/(m-K) @ 0°C (grey)	[105]
	50.2 @ 25°C (grey)	[105]
Electrical resistivity:	2.6x10 <sup>-7</sup> MOhm-m @ 0°C	[10]
	2.9x10 <sup>-13</sup> @ 22°C	[105]
Critical temperature:	803.°C	[47]
Critical pressure:	34.6 MPa	[47]
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	0.0050 K <sup>-1</sup> @ 20°C	[48]
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	NA	
Ionization potential:	9.81 eV (VUS)	[10], [105]
Magnetic volume susceptibility:	-69.0x10 <sup>-6</sup> SI units @ 20°C ( $\alpha$ )	[105]
	-297.8x10 <sup>-6</sup> @ 20°C ( $\beta$ )	[105]
	289.0x10 <sup>-6</sup> @ 20°C ( $\gamma$ )	[105]
Speed of sound:	unknown	
Heat of melting:	27.72 kJ/mol	[105]
	21.35	[10]
Heat of vaporization:	unknown	
Heat of sublimation:	31.95 kJ/mol	[10]



Heat capacity @ 25°C: 0.0247 kJ/(mol-K) (gray sol)[10],[105]  
 Heat of combustion: unknown  
 Heat of formation: 0.0 kJ/mol @ 25°C (gray sol)[10],[105]  
 14.7 (yellow sol)[10],[105]  
 4.19 (black amorphous)[10],[105]  
 Gibbs (free) energy: 0.0 kJ/mol (gray sol) [10]

Analytical chemistry:  $pP_{oct}$  = NA  
 $pK_s$  = NA  
 $pK_a$  = NA  
 $pK_{BH}$  = NA  
 Henry's law constant = NA  
 Hydrolysis half-life = NA

Electrochemical data: Tomilov and Chomutov (1974)

Clay-organic interaction data: inorganic

Solubility: Insoluble in water, caustic and nonoxidizing acids. Soluble in  $HNO_3$ . [22],[51]

Form: Silvery to black, brittle, crystalline or amorphous metalloid.  $\alpha$ -arsenic is the gray rhombohedral crystalline form.  $\beta$ -arsenic is the black amorphous form.  $\gamma$ -arsenic is the yellow cubic crystalline form. Rarely found in pure form but most commonly as arsenide of true metals. Can be heated to burn in air giving off an odor of garlic. Hardness 3.5 on the Mohs' scale. Valence states are -3, 0, +3, +5. Atomic number is 33 (Group VA). No stable isotopes. Technical grades are 90-95% pure; refined grades 99%; semiconductor grades 99.999%. [51],[10],[105],[108],[22]

Use: Hardening of lead shot and lead-base bearing materials; improve toughness and corrosion resistance of copper; the artificial isotope  $^{76}As$  as a radioactive tracer in toxicology; arsenates and arsenites used in agriculture as insecticides, herbicides, larvicides, and pesticides; arsenic trichloride in pharmaceuticals; other arsenic compounds are used in pigment production, manufacture of glass as a bronzing or decolorizing agent, manufacture of opal glass and enamels, textile printing, tanning, taxidermy, antifouling paints; high-purity grade used in the semi-conductor industry to make gallium arsenide for dipoles and other electronic devices, as a doping agent in germanium and silicon solid state, and as special solders. [108],[56],[22]

Fire and explosion hazard: Low

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable solid except when in the form of dust. Low fire hazard in the form of dust when exposed to heat or flame or by chemical reaction with powerful oxidizers. Slight explosion hazard in the form of dust when exposed to flame. Emits highly toxic fumes of arsenic oxides when heated or in contact with acid or acid fumes. Fight fire with  $CO_2$ , dry chemical powder, alcohol or polymer foam. [51],[55]

## 122 - Arsenic

**Incompatibility:** Acids; acid fumes; oxidizers; bromates; chlorates; iodates; peroxides; halogens; zinc; palladium; platinum; Li;  $\text{NCl}_3$ ;  $\text{KNO}_3$ ;  $\text{KMnO}_4$ ;  $\text{Rb}_2\text{C}_2$ ;  $\text{AgNO}_3$ ;  $\text{NOCl}$ ;  $\text{IF}_5$ ;  $\text{CrO}_3$ ;  $\text{ClF}_3$ ;  $\text{ClO}$ ;  $\text{BrF}_3$ ;  $\text{BrF}_5$ ;  $\text{BrN}_3$ ;  $\text{RbC}\equiv\text{CH}$ ;  $\text{CsC}\equiv\text{CH}$ ;  $\text{Na}_2\text{O}_2$ ; hexafluoro isopropyl ideneamino lithium; heat; air sensitive. [51],[55]

**Handling:** WARNING: avoid all contact. Keep away from heat and open flame when in the form of dust. Do not breathe dust or fumes (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (chemical resistant gloves and suit; safety goggles or face shield). Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [55],[56]

**Health effects:** Arsenic is highly poisonous and a carcinogen. Routes of entry are inhalation, ingestion of dust and fumes, skin absorption, and eye and skin contact. Points of attack include skin, eyes, and respiratory system. Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. onset may be delayed 2 to 4 hours or longer. Acute symptoms following ingestion include nausea, vomiting and diarrhea which can proceed to shock and death. Chronic exposure can result in skin exfoliation and pigmentation, herpes, polyneuritis, altered hematopoiesis, degeneration of liver and kidneys. Inhalation of inorganic arsenic compounds is the most common cause of chronic poisoning in the industrial situation. At first, the worker may complain of weakness, loss of appetite, some nausea, occasional vomiting, a sense of heaviness in the stomach, and diarrhea. Then the worker may complain of conjunctivitis, a catarrhal state of the mucous membranes of the nose, larynx, and respiratory passages. Coryza, hoarseness, and mild tracheobronchitis may occur. Perforation of the septum, skin lesions are common. Skin cancer is causally associated with exposure to inorganic arsenic compounds in drugs, drinking water and the occupational environment. It has been used as a food additive for human consumption. [51],[56],[55],[61]

**Toxicity:** Very high.

TWA: 0.065 ppm (0.2 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: 2 µg/m<sup>3</sup> [51]

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: potential human carcinogen [51],[108],[56],[22]

human, sufficient evidence (IARC cancer review) [55]

Mutagenicity: possible [51]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: 7857 mg/kg body wt for 55 yrs -- systemic skin and  
gastrointestinal tract effects [51]

Lethal: unknown

Inhalation: unknown

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown

## 124 - Benz(e)acephenanthrylene

Benz(e)acephenanthrylene

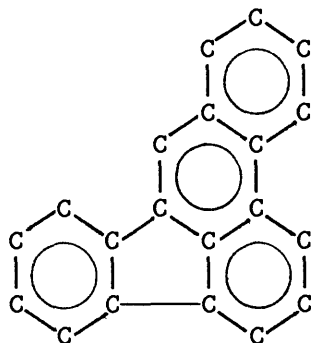
C<sub>20</sub>H<sub>12</sub>

CAS RN: 205-99-2

Syn: Benz(e)acephenanthrylene \* BbFL \* BbF \* 3,4-Benz(e)acephenanthrylene  
 \* 2,3-Benzfluoranthene \* 3,4-Benzfluoranthene \* Benzo(b)fluoranthene \*  
 Benzo(e)fluoranthene \* 2,3-Benzofluoranthene \* 3,4-Benzofluoranthene \* 2,3-  
 Benzofluoranthrene \* B(b)F \*

Structural formula:

Polynuclear Aromatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	252.315	
Specific gravity:	unknown	
Boiling point:	481.°C	[59]
Melting point:	168.°C	[106], [105]
Refractive index:	unknown	
Vapor pressure:	7.x10 <sup>-8</sup> kPa @ 20°C (5x10 <sup>-7</sup> mm)	[31], [41]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	4.4 μm <sup>2</sup> /s (calculated)	[59]
Solution diffusivity:	0.47 nm <sup>2</sup> /s (calculated)	[59]
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	unknown	
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	unknown	
Heat of combustion:	unknown	
Heat of formation:	unknown	

Gibbs (free) energy:	418.7 kJ/mol (gas) (calculated)	[59]
Analytical chemistry: pP <sub>oct</sub> =	6.57	[41],[59],[8]
	6.06	[31]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	>15.	[59]
	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	0.00122 kPa·m <sup>3</sup> /mol	[41]
	0.699 dimensionless (calc)	[59]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water. Slightly soluble in benzene.  
Soluble in most solvents. [105],[41]

0.0001 wt% in water [59]

0.0000012 wt% in water @ 25°C [41]

Form: Crystalline solid. Off-white fibers. [106],[55]

Use: There is no commercial-scale production. Present in crude oil, lubricating oils, gasoline engine exhaust, cigarette smoke, sewage sludge, effluent. [104]

Fire and explosion hazard: Unknown

Flash point: unknown

uel: unknown

lel: unknown

Autoign. temp.: unknown

Emits acrid smoke and irritating fumes, including CO and CO<sub>2</sub>, when heated to decomposition. Fight fire with water spray, carbon dioxide, dry chemical powder, alcohol or polymer foam. [51],[55]

Incompatibility: Strong oxidizing agents. [55]

Handling: WARNING: avoid all contact. Do not breathe dust or fumes (appropriate respirator or self-contained breathing apparatus). Do not allow skin or eye contact (chemical resistant gloves, safety goggles, other protective clothing). Use in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [51],[55]

Health effects: B(p)F is an irritant and potential human carcinogen. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. The chemical, physical, and toxicological properties have not been thoroughly investigated. A common air contaminant.  
[104],[51],[55]

**126 - Benz(e)acephenanthrylene**

**Toxicity:** Unknown

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: NA

Odor threshold: unknown

Carcinogenicity: positive animal determination [51]

animal sufficient evidence (IARC review) [55]

Mutagenicity: equivocal tumorigenic agent by RTECS criteria [55]

**Exposure:** Unknown

Benz[a]anthracene

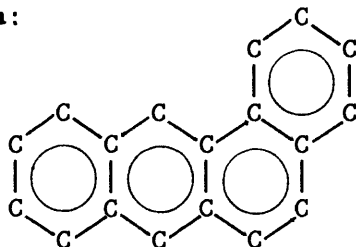
C<sub>18</sub>H<sub>12</sub>

CAS RN: 56-55-3

Syn: Benz[a]anthracene \* B(a)A \* BA \* Benzanthracene \* 1,2-Benz(a)anthracene \* 1,2-Benzanthracene \* Benzanthrene \* 1,2-Benzanthrene \* Benzo(a)anthracene \* Benzoanthracene \* 1,2-Benzoanthracene \* Benzo(a)phenanthrene \* Benzo(b)phenanthrene \* 2,3-Benzophenanthrene \* 2,3-Benzphenanthrene \* Naphthanthracene \* RCRA Waste Number U018 \* Tetraphene \*

Structural formula:

Polynuclear Aromatic Hydrocarbon



Physical properties:

Relative molecular mass:	228.293	
Specific gravity:	1.274	[41]
	1.174	[59]
Boiling point:	400.°C	[51]
	435.°C sublimes	[105], [106]
	437.6°C	[10]
Melting point:	162.°C	[105], [106]
	160.°C	[51]
	159.°-160°C sublimes	[10]
	155.°-157°C sublimes	[56]
Refractive index:	NA	
Vapor pressure:	1.35x10 <sup>-6</sup> kPa @ 20°C (1x10 <sup>-5</sup> mm)	[8]
	6.5x10 <sup>-9</sup> @ 20°C (5x10 <sup>-8</sup> mm)	[31]
	6.5x10 <sup>-10</sup> @ 20°C (5x10 <sup>-9</sup> mm)	[59]
Vapor density:	unknown	
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	4.6 μm <sup>2</sup> /s	[59]
Solution diffusivity:	0.5 nm <sup>2</sup> /s	[59]
Electric dipole moment:	unknown	
Ionization potential:	8.01 eV (EI)	[105]
	7.45	[41]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	21.38 kJ/mol	[105]

## 128 - Benz[a]anthracene

Heat of vaporization: unknown  
Heat of sublimation: unknown  
Heat capacity @ 25°C: unknown  
Heat of combustion: unknown  
Heat of formation: 172. kJ/mol @ 25°C (sol) [10]  
Gibbs (free) energy: unknown

Analytical chemistry:  $pP_{oct}$  = 5.91 [41],[27]  
5.61 [59],[8],[31]  
 $pK_s$  = NA  
 $pK_a$  = >15. [59]  
NA [31]  
 $pK_{BH}$  = NA  
Henry's law constant = 0.00081 kPa-m<sup>3</sup>/mol [41]  
6.7x10<sup>-5</sup> [41]  
4.5x10<sup>-6</sup> dimensionless (calc) [59]  
Hydrolysis half-life = NA [8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water. Slightly soluble in hot ethanol, acetic acid. Soluble in acetone, ether, and other organic solvents. Very soluble in benzene. [10],[104],[105]

0.0000010 wt% in water [104]  
0.0000044 wt% practical grade in water  
@ 24°C [104]

Form: Colorless to yellow-brown leaflets or plates (solid). [51],[56],[106]

Use: BA is a contaminant with no reported commercial use or application. It is found in gasoline (0.04 mg/l to 0.272 mg/l) and automobile exhaust, crude oil, bitumen, wood preservative sludge, oil, waxes, smoke, charcoal broiled, barbecued or smoked meats, and drugs. [51],[104],[56]

Fire and explosion hazard: Unknown

Flash point: unknown

uel: unknown

lel: unknown

Autoign. temp.: unknown

Though no information was found, BA is probably nonflammable. Emits acrid smoke and irritating fumes, including carbon monoxide and carbon dioxide, when heated to decomposition. Fight fire with water spray, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [51],[55]

Incompatibility: Strong oxidizing agents. [55]

Handling: Appropriate respirator or self-contained breathing apparatus required if concentrations above TWA. Wear protective clothing to prevent any possibility of skin or eye contact (nitrile, neoprene, or PVA gloves and suit; splash-proof chemical goggles). Safety shower and eye bath should be available. Keep container tightly closed. Store in secure poison area. [53],[55]



**Health effects:** BA is a confirmed human carcinogen and irritant. Routes of entry are inhalation, ingestion, and absorption through skin. The chemical, physical, and toxicological properties have not been thoroughly investigated. [104],[1],[55],[89]

**Toxicity:** Very high

TWA: 0.02 ppm (0.2 mg/m<sup>3</sup>) -- confirmed carcinogen -- for coal tar pitch volatiles [1]

STEL: no value set for coal tar pitch volatiles [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: positive results in animals [104],[1]  
confirmed human carcinogen [104],[1]

Mutagenicity: suspected human mutagen [104]

**Exposure:** Unknown

## 130 - Benzene

Benzene

C<sub>6</sub>H<sub>6</sub>

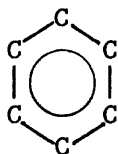
CAS RN: 71-43-2

Syn: Benzene \* (6)Annulene \* Benzol \* Benzole \* Benzolene \* Bicarburet of hydrogen \* Carbon oil \* Coal naphtha \* Cyclohexatriene \* Mineral naphtha \* Motor benzol \* NCI-C55276 \* Nitration benzene \* Phene \* Phenyl hydride \* Polystream \* Pyrobenzol \* Pyrobenzole \* RCRA Waste Number U019 \* UN 1114 (DOT) \*

Molecular formula: C<sub>6</sub>H<sub>6</sub>

Monocyclic Aromatic Hydrocarbon

Structural formula:



## Physical properties:

Relative molecular mass:	78.1136	
Specific gravity:	0.8794	[51]
	0.8790	[47], [22], [49]
	0.8786	[104]
	0.8765	[106], [105]
Boiling point:	80.1°C	[47], [22], [10], [107], [104], [105]
	80.094°C	[49]
	80.093°-80.094°C	[51]
Melting point:	5.533°C	[10], [49]
	5.51°C	[51]
	5.5°C	[106], [47], [20], [107], [104], [105]
Refractive index:	1.50112	[49]
	1.5011	[22], [105]
	1.4979	[10]
Vapor pressure:	1.33 kPa @ -11.5°C	(10mm) [20], [105]
	2.66 @ -2.6°C	(20mm) [20]
	5.33 @ 7.6°C	(40mm) [20], [105]
	8.0 @ 15°C	(60mm) [104]
	8.0 @ 15.4°C	(60mm) [47]
	10.13 @ 20°C	(76mm) [104], [47]
	12.7 @ 25°C	(95.2mm) [49]
	13.33 @ 26.1°C	(100mm) [51], [105]
	15.73 @ 30°C	(118mm) [104]
Vapor density:	2.77	[104], [51]
	2.7	[107]
Evaporation rate:	5.1	[49]
Relative dielectric permittivity:	2.284 @ 20°C	[20], [105]
	2.275 @ 25°C	[10], [105]
	2.27401 @ 25°C	[49]
	2.073 @ 129°C	[105]
Loss tangent	unknown	
Relaxation time:	unknown	

Thermal conductivity:	0.139 W/(mol-K) @ 12°C	[10]	
	0.146 @ 20°C	[20]	
	0.159 @ 30°C	[47]	
	0.141 @ 40°C	[20]	
	0.136 @ 60°C	[20]	
	0.151 @ 60°C	[47]	
Electrical resistivity:	1316. MOhm-m	[10]	
Critical temperature:	289.5°C	[20]	
	289.01°C	[49]	
	288.94°C	[10]	
	288.9°C	[107]	
	288.5°C	[47]	
Critical pressure:	4.92 MPa	[20]	
	4.898	[10], [49]	
	4.89	[107]	
	4.83	[47]	
Dynamic viscosity:	0.912 mPa-s @ 0°C	[105]	
	0.758 @ 10°C	[105]	
	0.652 @ 20°C	[105]	
	0.6028 @ 25°C	[10]	
	0.564 @ 30°C	[105]	
	0.503 @ 40°C	[105]	
	0.442 @ 50°C	[105]	
Kinematic viscosity:	1.041 μm²/s @ 0°C		
	0.865 @ 10°C		
	0.744 @ 20°C		
	0.6857 @ 25°C		
	0.643 @ 30°C		
	0.574 @ 40°C		
	0.504 @ 50°C		
Surface tension:	30.22 mN/m @ 10°C air	[20], [105]	
	28.85 @ 20°C air	[49], [105]	
	28.9 @ 20°C	[107]	
	28.20 @ 25°C	[49]	
	27.56 @ 30°C air	[22], [49], [105]	
	26.14 @ 40°C	[14]	
Contact angle: [18]			
	sessile	advancing	receding
quartz	12	18	6
calcite	18	23	9
biotite	10	19	7
Ca-mont.	9	swelled	swelled
Thermal expansion coefficient:	0.001213 K <sup>-1</sup>	[49]	
Compressibility:	0.864 nPa <sup>-1</sup> @ 10°C	[105]	
	0.937 @ 20°C	[105]	
	0.966 @ 25°C	[49]	
	1.012 @ 30°C	[105]	
	1.096 @ 40°C	[105]	
Vapor diffusivity:	7.7 μm²/s @ 0°C	[47]	
Solution diffusivity:	1.09 nm²/s in water @ 25°C	[59]	
	1.53 in CCl <sub>4</sub>	[47]	
Electric dipole moment:	0.	[10]	
Ionization potential:	9.24 eV (S,PI)	[105]	

## 132 - Benzene

Magnetic volume susceptibility:	-7.68x10 <sup>-6</sup> SI units	[105]
Speed of sound:	1295. m/s @ 25°C	[105]
	1310. @ 25°C	[20]
Heat of melting:	9.958 kJ/mol	[107]
	9.951	[105]
	9.872	[10]
	9.866	[49]
Heat of vaporization:	42.93 kJ/mol	[105]
	34.11	[105]
	33.87	[10]
	30.78	[107]
	30.726	[49]
Heat of sublimation:	44.572 kJ/mol	[49]
	33.87	[10]
Heat capacity @ 25°C:	0.1356 kJ/(mol-K) (liq)	[105]
	0.135760 (liq)	[49]
	0.0817 (gas)	[10]
	0.0816 (gas)	[105]
Heat of combustion:	-3269.7 kJ/mol @ 25°C (liq)	[20], [105]
	-3267.58 (liq)	[49]
	-3303.6 (gas)	[20]
Heat of formation:	49.03 kJ/mol @ 25°C (liq)	[20], [10]
	49.028 (liq)	[49]
	82.98 (gas)	[10]
	82.89 (gas)	[49], [20]
Gibbs (free) energy:	124.4 kJ/mol @ 25°C (liq)	[10]
	129.7 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	2.13 @ 20°C	[104], [12], [21], [31], [59]
	2.12	[4], [27]
	1.95	[8]
	1.56	[21]
	pK <sub>s</sub> unknown	
	pK <sub>a</sub> =	>15. [59]
	pK <sub>BH</sub> =	9.4 [49]
Henry's law constant =	0.555 kPa-m <sup>3</sup> /mol @ 25°C	[41]
	0.550	[24]
	0.227 dimensionless	[59]
Hydrolysis half-life =	NA	[8]

**Electrochemical data:** Loveland and Dimeler (1961), Pysh and Yang (1963), Hansen et al. (1964), Neikam and Desmond (1964), Shriver et al. (1964), Osa and Kuwana (1969), Meites and Zuman (1977), Meites et al. (1977b), Nyberg (1978), Anderson and Stocker (1983), Eberson and Utley (1983a), Lund (1983a), Meites et al. (1983)

**Clay-organic interaction data:** Benzene decreases the hydraulic conductivity of kaolinite clay soils (Acar et al., 1984, 1985). Absorption by montmorillonite and vermiculite samples previously dehydrated at 293 K. Intercalation by montmorillonite saturated with  $\text{Cu}^{2+}$ . Increase in basal spacing of montmorillonite and hectorite complexes with a series of alkylammonium ions on intercalation of benzene (see also [18]). Frequencies of C-C stretching and C-H out-of-plane vibrations of benzene in the liquid state and when adsorbed by  $\text{Cu(II)montmorillonite}$ . (Theng, 1974). Also see Acar et al., 1984, 1985; Barshad, 1952; Chiou et al., 1983; Doner and Mortland, 1969; Greene-Kelly, 1955; Karickhoff et al., 1979; Pinnavaia and Mortland, 1971; Rodgers et al., 1980; Serratos, 1968; Vandepoel et al., 1973.

**Solubility:** Slightly soluble in water. Miscible with ethanol, ether, acetone, chloroform, carbon disulfide, carbon tetrachloride, glacial acetic acid, oils and most organic solvents. [10],[22],[105]

0.178 wt% in water @ 20°C [104]

0.07 wt% in water @ 22°C [10],[47]

0.1791 wt% in water @ 25°C [49]

**Form:** Clear, colorless liquid. Characteristic gasoline-like aromatic odor. Commercial grades may contain up to 50% toluene, xylene and other constituents which distill below 120°C. [22],[51],[56]

**Use:** Manufacture of medicinal chemicals, polymers detergents, pesticides, dyes and many other organic compounds, artificial leather, linoleum, oil cloth, airplane dopes, varnishes, lacquers; solvent for waxes, resins, oils, etc.; antiknock gasolines (1.8-5 vol% [104]); primary raw material for styrene used in synthetic rubber, for nylon intermediates, for phenol, and for synthetic detergents; coal tar distillation; coal processing; coal coking; extraction of oils from seeds and nuts. Thirteenth in order of high-volume chemicals produced in U.S. (1975). Benzene is present in gasoline engine exhaust from 0.1 to 42.6 ppm. [56],[104]

**Fire and explosion hazard:** Very high.

Flash point: (CC) -11°C [51],[107],[49],[22]

uel: 9.1% [10]

8.0% [22],[51]

7.9% [107]

lel: 1.5% [22]

1.4% [51]

1.3% [107]

1.2% [10]

Autoign. temp.: 592°C [107]

562°C [51],[22]

Volatile, extremely flammable liquid. Dangerous fire hazard when exposed to heat, sparks or flame. Flashback along vapor trail may occur. Can react vigorously with oxidizing materials. Moderate explosion hazard when vapors are exposed to flame. May emit hazardous fumes of CO and  $\text{CO}_2$  when heated to decomposition. Fight fire with alcohol or polymer foam,  $\text{CO}_2$  or dry chemical powder. Water may be ineffective. Use water spray to cool fire-exposed containers. [51],[107],[55]

## 134 - Benzene

**Incompatibility:** Oxidizing materials;  $\text{BrF}_3$ ,  $\text{Cl}_2$ ,  $\text{CrO}_3$ ,  $\text{O}_2\text{NClO}_4$ ,  $\text{O}_2$ ,  $\text{O}_3$ , perchlorates,  $(\text{AlCl}_3+\text{FeClO}_4)$ ,  $(\text{H}_2\text{SO}_4+\text{permanganates})$ ,  $\text{K}_2\text{O}_2$ ,  $(\text{AgClO}_4+\text{acetic acid})$ ,  $\text{Na}_2\text{O}_2$ , boron hydride, sulfuric acid, nitric acid; chlorine, bromine with iron, diborane. [56]

**Handling:** Avoid heat, flame and sources of ignition. Use with adequate ventilation (fume hood). Appropriate respirator required. Self-contained breathing apparatus recommended. Do not allow skin contact (PVA synthetic latex gloves; lab coat, chemical goggles or face shield). Safety shower and eye bath should be available. Keep container tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet. Should not use glass containers for storage. Store in secure poison area. [56],[107],[53]

**Health effects:** Benzene is a poison and a carcinogen. Routes of entry are inhalation of vapor, absorption through skin, ingestion, and skin and eye contact. Points of attack include blood, central nervous system, skin, bone marrow, eyes, and respiratory system, gastrointestinal system. Locally, benzene has a comparatively strong irritant effect to the eyes, nose and throat, producing erythema and burning, and, in more severe cases, edema and even blistering. Symptoms of overexposure include allergic sensitization, CNS effects (restlessness, convulsions, excitement, depression), peripheral nervous system effects, blood cell disorders, immunological effects, and gastrointestinal effects. Benzene has a definite cumulative action, and exposure to relatively high concentrations is not serious from the point of view of causing damage to the blood-forming system, provided the exposure is not repeated. Benzene is a common air contaminant. [56],[51],[62]

**Toxicity:** Moderate.

TWA: 10 ppm (30  $\text{mg}/\text{m}^3$ ) [1]

STEL: no value set [1]

CL: 25 ppm (80  $\text{mg}/\text{m}^3$ ) [51]

IDLH: 2000 ppm (6390  $\text{mg}/\text{m}^3$ ) [107],[56]

Peak: 50 ppm (160  $\text{mg}/\text{m}^3$ ) for 10 min [51]

Odor threshold: 4.68 ppm (15  $\text{mg}/\text{m}^3$ ) [107]

0.2-320 ppm (0.6-1020  $\text{mg}/\text{m}^3$ ) [104]

**Carcinogenicity:** Listed as a carcinogen by the EPA. Noted as a suspected human carcinogen by ACGIH. [51],[56],[1] positive [25],[26],[34]

**Mutagenicity:** indefinite [62]

**Exposure:****External:**

Non-lethal: unknown

Lethal: unknown

**Oral:**

Non-lethal: 130 mg/kg body wt -- CNS effects [51]

Lethal dose: 194 mg/kg body wt -- death of an adult male [51]  
50-500 mg/kg [107]**Inhalation:**Short-term Inhalation limits: 75 ppm (240 mg/m<sup>3</sup>) for 30 min [107]Non-lethal: >50 ppm (160 mg/m<sup>3</sup>) -- unsatisfactory [104]

100 ppm for 10 yrs at int. -- carcinogenic effects [51]

100 ppm (300 mg/m<sup>3</sup>) -- CNS effects [51]210 ppm (670 mg/m<sup>3</sup>) -- blood effects [51]

400 ppm/8 yrs at int. -- equivocal tumorigenic effect [51]

500 ppm (1500 mg/m<sup>3</sup>) -- symptoms of illness [104]

650 ppm/4 yrs at int. -- carcinogenic effects [51]

1500 ppm (4.5 g/m<sup>3</sup>) for 60 min -- severe toxic effects [104]Lethal: 20000 ppm (60 g/m<sup>3</sup>)/5 min -- death of an adult human [51]

## 136 - Benzidine

Benzidine

 $C_{12}H_{12}N_2$ 

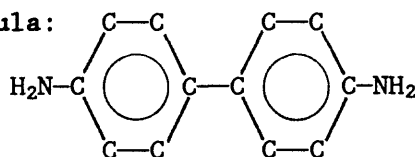
CAS RN: 92-87-5

Syn: Benzidine \* [1,1'-Biphenyl]-4,4'-diamine \* Benzidine base \* *p,p'*-Bianiline \* *P,P'*-Bianiline \* 4,4'-Bianiline \* Biphenyl, 4,4'-diamino- \* 4,4'-Biphenyldiamine \* 4,4'-Biphenylenediamine \* C.I. 37225 \* C.I. azoic diazo component 112 \* 4,4'-Diaminobiphenyl \* *p,p'*-Diaminobiphenyl \* 4,4'-Diamino-1,1'-biphenyl \* *p*-Diaminodiphenyl \* *para*-Diaminodiphenyl \* 4,4'-Diaminodiphenyl \* *p,p'*-Dianiline \* 4,4'-Diphenylenediamine \* Fast Corinth Base B \* NCI-C03361 \* RCRA Waste Number U021 \* UN 1885 (DOT) \*

Molecular formula:  $NH_2-C_6H_4-C_6H_4-NH_2$ 

Aromatic Polyamine

Structural formula:



## Physical properties:

Relative molecular mass:	184.241	
Specific gravity:	1.250	[104], [51]
Boiling point:	402.°C	[104]
	401.7°C	[51]
Melting point:	129.°C	[104]
	128.°C	[10]
	127.°C	[22]
	125.°C	[106]
	122.°-128°C	[105]
	116.°C	[104]
Refractive index:	unknown	
Vapor pressure:	0.133 kPa @ -4°C (1mm)	[105]
	1.333 kPa @ 30°C (10mm)	[105]
Vapor density:	6.36	[104]
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	2.98 $\mu m^2/s$ @ 0°C	[47]
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	-9.48x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	unknown	





## 138 - Benzidine

**Handling:** Prohibit contact in any manner. Any exposure is considered extremely hazardous. Avoid heat. Do not inhale dust, mist, or fumes (self-contained breathing apparatus required). Prevent all contact with eyes, skin, or clothing (fully-encapsulating protective clothing). Skin absorption may be significant. In case of contact, immediately wash skin with plenty of soap and water. Flush eyes with plenty of water for at least 15 minutes. Get medical attention at once. Immediately remove all contaminated clothing and leave at the site. Keep container tightly closed and protected from light. Store in cool, dry, secure poison area or cabinet. [51],[56],[108]

**Health effects:** Benzidine is a poison and confirmed human carcinogen. Avoid all contact. Any exposure is considered extremely hazardous. Routes of entry are inhalation, percutaneous absorption, and ingestion of dust. Points of attack are skin, blood, bladder, and respiratory tract. It can cause damage to the blood including hemolysis and bone marrow depression. On ingestion, causes nausea and vomiting and may result in liver and kidney damage. Other symptoms of exposure can include painful and irregular urination. It is a known human urinary tract carcinogen with an average 16 year latent period. The first symptoms of bladder cancer usually are hematuria, frequency of urination, or pain. [51],[56],[108],[55]

**Toxicity:** Very high

TWA: no values set (skin) -- confirmed human carcinogen [1]

STEL: no values set (skin) -- confirmed human carcinogen [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: human positive [51],[56],[104],[1]

Mutagenicity: potential mutagen [51],[104]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: 2.4 ppm (18 mg/m<sup>3</sup>) intermit. for 13 yrs -- carcinogenic effects [51]

Lethal: unknown

Benzoic acid

 $C_7H_6O_2$ 

CAS RN: 65-85-0

Syn: Benzoic acid \* Benzenecarboxylic acid \* Benzeneformic acid \*  
 Benzenemethanoic acid \* Benzoate \* Carboxybenzene \* Carboxyl benzene \*  
 Draclyic acid \* NA 9094 (DOT) \* Phenylcarboxylic acid \* Phenylformic acid  
 Retarder BA \* Retardex \* Salvo liquid \* Salvo powder \* Tenn-plas \*

Molecular formula:  $C_6H_5COOH$ 

Aromatic Carboxylic Acid

**Physical properties:**

Relative molecular mass:	122.123	
Specific gravity:	1.27	[104]
	1.080	[10]
	1.266 @ 15/4	[47]
	1.2659 @ 15/4	[105], [22], [106]
	1.316 @ 28/4	[51], [107]
Boiling point:	249.2°C	[107], [22], [47]
	249.°C	[105], [51], [104]
Melting point:	122.4°C	[10], [56], [106]
	122.3°C	[107]
	122.13°C	[105]
	121.7°C	[51], [104], [47]
	121.25°C	[22]
	>100.°C (sublimes)	[10], [22]
Refractive index:	1.504 @ 32°C	[105], [106]
Vapor pressure:	0.0006 kpa @ 20°C (0.0045mm)	[23]
	0.133 @ 96°C (1mm)	[51], [105]
	1.33 @ 132°C (10mm)	[55]
Vapor density:	4.21	[51], [104]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	3.3 MOhm-m @ 125°C	[10], [11]
Critical temperature:	479.°C	[107]
Critical pressure:	4.56 MPa	[107]
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	2.62 nm <sup>2</sup> /s in acetone	[47]
	1.38 in benzene	[47]
	0.91 in CCl <sub>4</sub>	[47]
	0.043 in ethylene glycol	[47]
	1.49 in toluene	[47]
Electric dipole moment:	unknown	
Ionization potential:	9.73 eV (EI)	[105]
Magnetic volume susceptibility:	-9.15x10 <sup>-6</sup> SI units @ 15°C	[105]
Speed of sound:	unknown	

## 140 - Benzoic acid

Heat of melting:	17.32 kJ/mol	[105]
	17.174	[107]
	18.09	[10]
Heat of vaporization:	63.863 kJ/mol	[105]
	68.224	[105]
	50.66	[10]
Heat of sublimation:	95.04 kJ/mol	[10]
Heat capacity @ 25°C:	0.1464 kJ/ (mol-K) (sol)	[10]
Heat of combustion:	-3229.03 kJ/mol @ 25°C (liq)	[105]
Heat of formation:	-385.3 kJ/mol @ 25°C (sol)	[10]
Gibbs (free) energy:	-245.4 kJ/mol @ 25°C (sol)	[10]

Analytical chemistry:	P <sub>oct</sub> =	2.03	[41], [21]
		1.87 @ 20°C	[104], [23], [21], [27]
	pK <sub>s</sub> =	unknown	
	pK <sub>a</sub> =	4.205 @ 20°C	[11], [23]
		4.204 @ 25°C	[10]
		4.201 @ 25°C	[11]
		4.19 @ 25°C	[105], [108]
		4.203 @ 30°C	[11]
		4.205 @ 35°C	[11]
	pK <sub>BH</sub> =	unknown	
	Henry's law constant =	7.11x10 <sup>-6</sup> kPa-m <sup>3</sup> /mol (calc)	[41]
	Hydrolysis half-life =	unknown	

**Electrochemical data:** Meites and Zuman (1977), Meites et al. (1977b), Meites et al. (1983)

**Clay-organic interaction data:** Yariv et al. (1966)

**Solubility:** Slightly soluble in water, ligroin. Soluble in acetone, benzene, carbon tetrachloride, toluene, chloroform, ethanol, methanol, hot water, carbon disulfide, turpentine. Very soluble in ether, acetone, hot benzene. Solubility in water is increased by alkaline substances.

[105], [22], [108]

0.17 wt% in water @ 0°C	[108]
0.21 wt% in water @ 10°C	[108]
0.27 wt% in water @ 18°C	[104], [23]
0.2 vol% in water @ 17°C	[47]
0.21 wt% in water @ 17.5°C	[10]
0.29 wt% in water @ 20°C	[108]
0.34 wt% in water @ 25°C	[108]
0.42 wt% in water @ 30°C	[108]
0.60 wt% in water @ 40°C	[108]
0.95 wt% in water @ 50°C	[108]
46. vol% in ethanol @ 15°C	[47]
46.6 wt% in ethanol @ 15°C	[10]
66. vol% in ether @ 15°C	[47]

1. g in 4.5 ml chloroform	[108]
1. g in 3 ml ether	[108]
1. g in 3 ml acetone	[108]
1. g in 30 ml CCl <sub>4</sub>	[108]
1. g in 10 ml benzene	[108]
1. g in 30 ml carbon disulfide	[108]
1. g in 23 ml oil of turpentine	[108]

**Form:** White scales, needle crystals, or powder. Faint, pleasant, slightly aromatic odor of benzoin or benzaldehyde. [107],[22],[104]

**Use:** Preserving foods, fats, fruit juices, alkaloid solutions (restricted to 0.1%); pharmaceutical and cosmetic preparations; manufacturing of alkyl resins; intermediate in the synthesis of dyestuffs and pharmaceuticals; production of phenol, sodium and butyl benzoates, and caprolactam; plasticizer manufacturing to modify PVC resins, PV acetate and phenol-formaldehyde; seasoning tobacco; germicide; perfumes; a mordant in calico printing. Naturally occurs in cranberries, prunes, ripe cloves, bark of wild black cherry tree, scent glands of beavers, and oil of anise seeds. [22],[56],[104],[108]

**Fire and explosion hazard:** Low.

Flash point: (CC) 121°C [107],[51],[107],[22]

uel: unknown

lel: unknown

Autoign. temp.: 572.8°C [107]

571.1°C [51]

Slightly flammable solid. Slight fire and explosion hazard. Concentrated dust, or vapor from molten benzoic acid, may form explosive mixture in air, specially in an enclosed area. Emits acrid smoke and irritating fumes, such as carbon monoxide and carbon dioxide, when heated to decomposition. Fight fire with dry chemical powder, alcohol or polymer foam, water fog, CO<sub>2</sub>. [51],[107],[55]

**Incompatibility:** Strong oxidizing agents; strong bases; strong reducing agents. [51],[55]

**Handling:** Avoid personal contact with solid or dust. Appropriate respiratory or self-contained breathing apparatus should be worn to prevent inhalation. Prevent skin and eye contact (neoprene or nitrile protective outer wear; splash-proof safety goggles). Safety shower and eye bath should be available. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [107],[53],[55]

**Health effects:** Benzoic acid is a mild irritant. Routes of entry are inhalation and ingestion. Points of attack include skin, eyes, mucous membranes, respiratory system, and gastrointestinal system. It is mildly irritating to the skin, eyes, and mucous membranes. Dust may be irritating to the eyes and nose. At elevated temperatures, fumes may cause irritation of the eyes, respiratory system and skin. Ingestion may cause nausea and gastrointestinal tract problems. [51],[107],[56]

142 - Benzoic acid

**Toxicity:** Very low.

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: none [104]

Mutagenicity: none [104]

**Exposure:**

External:

Non-lethal: 22 mg intermit. for 3 days -- moderate skin irritation [51]

6 mg/kg -- toxic skin effects [51]

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: 500 mg/kg body wt -- death of an adult male [51]

0.5-5 g/kg body wt [107]

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown

Benzo[a]pyrene

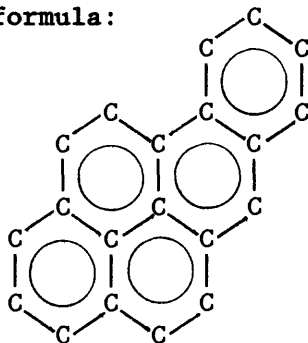
C<sub>20</sub>H<sub>12</sub>

CAS RN: 50-32-8

Syn: Benzo[a]pyrene \* Benzo(d,e,f)chrysene \* 1,2-benzpyrene \* 1,2-benzopyrene \* 3,4-Benzopyrene \* 6,7-Benzopyrene \* Benz(a)pyrene \* 3,4-Benz(a)pyrene \* 3,4-Benzopyrene \* BP \* 3,4-BP\* B(a)P \* RCRA Waste Number U022 \*

Structural formula:

Polycyclic Aromatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	252.315	
Specific gravity:	1.351	[41]
Boiling point:	495.°C	[41], [55]
	312.°C @ 10 mm Hg	[51]
	311.°C @ 10 mm Hg	[104]
	310.°-312°C @ 10 mm Hg	[105], [22]
Melting point:	179.°C	[104], [51], [22], [56]
	176.5°-177.5°C	[105]
	175.°C	[55]
Refractive index:	NA	
Vapor pressure:	7.5x10 <sup>-10</sup> kPa @ 25°C (5.6x10 <sup>-9</sup> mm)	[31]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	4.6 μm <sup>2</sup> /s	[59]
Solution diffusivity:	0.48 nm <sup>2</sup> /s in water	[59]
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	17.32 kJ/mol	[105]
Heat of vaporization:	unknown	

## 144 - Benzo[a]pyrene

Heat of sublimation: unknown  
Heat capacity @ 25°C: unknown  
Heat of combustion: unknown  
Heat of formation: unknown  
Gibbs (free) energy: 427.30 kJ/mol (gas) [59]

Analytical chemistry:  $pP_{oct}$  = 6.50 [41]  
6.06 [31]  
6.04 [41], [8]  
5.99 [41]  
5.97 [59]  
5.81 [41]  
 $pK_s$  = NA  
 $pK_a$  = >15. [59]  
NA [31]  
 $pK_{BH}$  = NA  
Henry's law constant =  $1.8 \times 10^{-5}$  dimensionless (calc) [59]  
Hydrolysis half-life = NA [8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water. Slightly soluble in ethanol.  
Soluble in benzene, toluene, xylene. [51], [22], [104]  
0.003 wt% in water [104]  
0.005-0.010 wt% in sea water @ 22°C [104]

Form: Yellowish crystalline powder. [51], [22], [55]

Use: There is no commercial-scale production. One U.S. company produces it in 100 mg to 5 g quantities for research. It is a by-product of combustion with 96% coming from commercial and residential coal burning, coke manufacturing, petroleum refining, shale refining, and kerosene processing. Present in coal tar, asphalt tarring operations, cigarette smoke (0.2-12.2  $\mu\text{g}/100$  cigarettes), food (0.1-50 ppb), and the atmosphere as product of incomplete combustion. See [104] for more complete listing of concentrations in food, smoke, fuels, etc. [22], [56], [104]

Fire and explosion hazard: Unknown

Flash point: unknown

uel: unknown

lel: unknown

Autoign. temp.: unknown

Emits acrid smoke and carbon monoxide and carbon dioxide when heated to decomposition. Fight fire with water spray,  $\text{CO}_2$ , dry chemical powder, alcohol or polymer foam. [51], [55]

Incompatibility: Oxidizing agents. [55]



**Handling:** Do not allow skin or eye contact or inhalation of dust or fumes (rubber boots and heavy rubber gloves; wear disposable coveralls and discard them after use). Wear protective clothing and appropriate respirator or self-contained breathing apparatus. Safety shower and eye bath should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [56],[22],[55]

**Health effects:** B(a)P is a suspected human carcinogen. Routes of entry are inhalation, ingestion, and skin absorption. Points of attack include brain and coverings, peripheral nervous system, upper respiratory system, gastrointestinal system, liver, kidney, ureter, bladder, blood, and skin. It may cause skin irritation. A common air contaminant in water, food, and smoke. The chemical, physical, and toxicological properties have apparently not been thoroughly investigated. [22],[51],[56],[55],[89]

**Toxicity:** Very high

TWA: Suspected human carcinogen [1]

STEL: Suspected human carcinogen [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: suspected human carcinogen; animal positive [51],[1]

Mutagenicity: experimental human mutagen and teratogen; DNA damage to HeLa and somatic mammalian cells [51]

**Exposure:**

External: unknown

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: 70 ng/m<sup>3</sup> cont. for a yr -- equivocal tumorigenic agent [51]

Lethal: unknown

## 146 - Beryllium

Beryllium

Be

CAS RN: 7440-41-7

Syn: Beryllium \* Be \* Beryllium-9 \* Glucinium \* Glucinum \* RCRA Waste  
 Number P015 \* UN 1567 (DOT) \*

Molecular formula: Be

Element

## Physical properties:

Relative molecular mass:	9.01218	[105]
Specific gravity:	1.85	[22], [107]
	1.848	[105]
	1.8477	[108]
Boiling point:	2970.°C @ 0.66 kPa (5mm)	[105]
	2970.°C	[47]
	2484.°C	[10]
Melting point:	1278.°C ± 5°C	[105]
	1278.°C	[47]
	1277.°C	[10]
Refractive index:	NA	
Vapor pressure:	0.133 kPa @ 1520°C (1mm)	[105]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	NA	
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	218. W/(m-K) @ 0°C	[105]
	201. @ 25°C	[105]
Electrical resistivity:	3.56x10 <sup>-14</sup> MOhm-m @ 20°C	[105]
	3.3x10 <sup>-14</sup> @ 22°C	[105]
	4.x10 <sup>-14</sup>	[45]
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	1100. mN.m @ 1500°C	[105]
Contact angle:	NA	
Thermal expansion coefficient:	0.000012 K <sup>-1</sup> @ 25°C	[105]
	0.0000130 @ 20°C	[48]
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	NA	
Ionization potential:	9.32 eV (VUS)	[105]
Magnetic volume susceptibility:	113.0x10 <sup>-6</sup> SI units	[105]
Speed of sound:	12890. m/s long. wave in bulk	[105]
	8880. shear wave in bulk	[105]
	12870. long. wave in thin rod	[105]
Heat of melting:	12.86 kJ/mol	[48]
	12.2	[105]
	11.7	[10]
	9.81	[105]
Heat of vaporization:	297.84 kJ/mol	[10]
	223.752	[48]
Heat of sublimation:	324.5 kJ/mol	[10]

Heat capacity @ 25°C:	0.0165 kJ/(mol-K) (sol)	[105],[10]
	0.01595 (liq)	[10]
	0.0208 (gas)	[10]
	0.01577 (sol)	[48]
@ 20°C:		
Heat of combustion:	-587.5 kJ/mol @ 25°C (sol)	[107]
Heat of formation:	0.0 kJ/mol @ 25°C (sol)	[105],[10]
	12.06 (liq)	[10]
	324.5 (gas)	[10]
	320.8 (gas)	[105]
Gibbs (free) energy:	0.0 kJ/mol @ 25°C (sol)	[10]
	9.965 (liq)	[10]
	286.8 (gas)	[10]

Analytical chemistry:  $pP_{oct}$  = NA  
 $pK_s$  = NA  
 $pK_a$  = unknown  
 $pK_{BH}$  = NA  
 Henry's law constant =  
 Hydrolysis half-life = NA

Electrochemical data: Chauvin and Coriou (1976)

Clay-organic interaction data: inorganic

**Solubility:** Insoluble cold water, mercury. Slightly soluble hot water.  
 Soluble in dilute acid or alkaline solutions. Decomposes.  
 [47],[105],[56],[10]

**Form:** Grayish-white, hard, light metal with hexagonal polycrystalline structure. Sweetish taste. It has an atomic number of 4 (group IIA -- alkaline earth metal) and valence of 2. Commercial grades of purity are Grade AA, 99.96+%, and Grade A, 99.87+%. [105],[51],[108]

**Use:** Alloying agent in producing beryllium copper, which is extensively used for springs, electrical contacts, spot-welding electrodes, and non-sparking tools; structural material for high-speed aircraft, missiles, and spacecraft; in nuclear reactors as a reflector or moderator because of its low thermal neutron cross section; used in gyroscopes, computer parts, and inertial guidance instruments where lightness, stiffness, and dimensional stability are required; manufacture of electrical components, chemicals, ceramics, special windows for X-ray tubes. It is also released through the burning of coal (250,000 pounds annually). [105],[56],[22],[5]

**Fire and explosion hazard:** Low.

Flash point: unknown

uel: unknown

lel: unknown

Autoign. temp.: unknown

Nonflammable solid. Combustible solid in the form of dust or powder. Moderate fire hazard in the form of dust or powder, or when exposed to flame or by spontaneous chemical reaction. Slight explosion hazard in the form of powder or dust. Emits very toxic fumes of BeO when heated to decomposition. May flash or spark on impact. Fight fire with graphite, sand, or any other inert powder. Stop discharge if possible. [51],[107]

## 148 - Beryllium

**Incompatibility:** Chlorinated hydrocarbons (such as  $\text{CCl}_4$  and  $\text{C}_2\text{HCl}_3$ ); lithium; phosphorous; halogens; halides; bases; acids; alkalies; oxidizable materials. [51],[56]

**Handling:** Avoid contact of dust or fumes with fire, heat, sparks, or sources of ignition. Prevent any reasonable possibility of inhalation of dust or fumes using appropriate respirator or self-contained breathing apparatus. Prevent any reasonable probability of skin and eye contact (rubber gloves and overclothing; chemical goggles). Clean clothing should be issued daily to site workers. Workers should shower before changing into street clothes. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [56],[57];[55]

**Health effects:** Beryllium and its salts are highly toxic. Beryllium itself is suspected human carcinogen and a poison. Routes of entry include inhalation of fumes or dust and skin contact. Points of attack include skin, eyes, respiratory system, lungs, liver, spleen, and heart. Compounds designated to be hazardous substances by the EPA include beryllium chloride, beryllium fluoride, and beryllium nitrate. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. Contact dermatitis of exposed parts of the body are caused by acid salts of beryllium. Eye irritation and conjunctivitis can occur. Exposure to soluble beryllium compounds may cause nasopharyngitis, a condition characterized by swollen and edematous mucous membranes, bleeding points, and ulceration. Acute systemic effects primarily involve the respiratory tract and are manifest by a nonproductive cough, substernal pain, moderate shortness of breath, and some weight loss. Symptoms may take 3 to 6 months to 5 to 10 years to develop. Symptoms of chronic exposure include respiratory symptoms, weakness, fatigue, and weight loss. [105],[51],[56],[5],[107],[5],[55]

**Toxicity:** High.

TWA: 0.005 ppm ( $2 \mu\text{g}/\text{m}^3$ ) -- suspected human carcinogen [1]

STEL: no value set [1]

CL: 0.014 ppm ( $5 \mu\text{g}/\text{m}^3$ ) [51]

0.0014 ppm ( $0.5 \mu\text{g}/\text{m}^3$ ) in a 130 min period -- recommended [51]

IDLH: unknown

Peak: 0.068 ppm ( $25 \mu\text{g}/\text{m}^3$ ) in an 8 hr period determined by >30 min sampling period [51],[56]

Odor threshold: odorless [107]

Carcinogenicity: experimental and suspected human [1]

positive animal [1],[51],[56]

human, limited evidence (IARC cancer review) [55]

Mutagenicity: experimental neoplastic effects [51]

equivocal tumorigenic agent (by RTECS criteria) [51],[55]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: 0.068 ppm (0.025 mg/m<sup>3</sup>) for less than  
30 min [107]

Non-lethal: 815 ppm (300 mg/m<sup>3</sup>) -- pulmonary system effects [51]

Lethal: unknown

# 150 - Bis(2-chloroethyl) ether

Bis(2-chloroethyl) ether

C<sub>4</sub>H<sub>8</sub>Cl<sub>2</sub>O

CAS RN: 111-44-4

Syn: Bis(2-chloroethyl) ether \* Ethane, 1,1'-oxybis[2-chloro- \* BCEE \*  
 bis( $\beta$ -chloroethyl) ether \* bis(chloro-2-ethyl) oxide \* Chlorex \* 1-Chloro-  
 2-( $\beta$ -chloroethoxy)ethane \* Chloroethyl ether \* 2-Chloroethyl ether \* DCEE  
 \* Dichloroether \* 2,2' Dichlorethyl ether \*  $\beta,\beta$ -Dichlorodiethyl ether \*  
 2,2'-Dichlorodiethyl ether \* Dichloroethyl ether \*  $\beta,\beta'$ -Dichloroethyl ether  
 \* 2,2'-Dichloroethyl ether \* sym-Dichloroethyl ether \* Di( $\beta$ -chloroethyl)  
 ether \* Di(2-chloroethyl) ether \* Dichloroethyl oxide \* ENT 4504 \* 1,1'-  
 Oxybis(2-chloro)ethane \* 1,1'-Oxibis[2-chloroethane] \* RCRA Waste Number  
 U025 \* UN 1916 (DOT) \*

Molecular formula: ClCH<sub>2</sub>CH<sub>2</sub>OCH<sub>2</sub>CH<sub>2</sub>Cl

Polychlorinated Aliphatic Open-Chain Ether

## Physical properties:

Relative molecular mass:	143.013	
Specific gravity:	1.22	[107], [104], [108]
	1.2199	[105]
	1.2192	[10], [49]
	1.2	[32]
Boiling point:	178.8°C	[10]
	178.75°C	[49]
	178.5°C	[51], [22]
	178.2°C	[32]
	178.°C	[105], [107], [104], [108], [106]
	176.°-178°C	[56]
Melting point:	-24.5°C	[105]
	-46.8°C	[105], [49]
	-50.°C	[104], [108], [106]
	-51.7°C	[10]
	-51.8°C	[22]
	-51.9°C	[51]
	-52.°C	[107]
Refractive index:	1.4575	[10], [105], [49]
	1.457	[22], [108]
	1.451	[106]
Vapor pressure:	0.0053 kPa @ 20°C	(0.4mm) [32]
	0.093 @ 20°C	(0.7mm) [51]
	0.095 @ 20°C	(0.71mm) [104]
	0.133 @ 23.5°C	(1mm) [105]
	0.187 @ 25°C	(1.4mm) [104]
	0.207 @ 25°C	(1.55mm) [49], [23]
	1.33 @ 62°C	(10mm) [105]
Vapor density:	4.93	[51], [107], [104]
	4.9	[32]
Evaporation rate:	0.1	[49]
Relative dielectric permittivity:	21.2 @ 20°C	[49], [11], [10]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	

Dynamic viscosity:	2.14 mPa-s @ 25°C	[10]
Kinematic viscosity:	1.75 $\mu\text{m}^2/\text{s}$ @ 25°C	
Surface tension:	38.61 mN/m @ 15°C	[10]
	37.9 @ 20°C	[107]
([10] and [49] values calculated)		
	37.96 @ 20°C	[10]
	37.6 @ 20°C	[49]
	37.31 @ 25°C	[10]
	37.0 @ 25°C	[49]
	36.65 @ 30°C	[10]
Contact angle:	unknown	
Thermal expansion coefficient:	0.00097 K <sup>-1</sup> @ 10°-30°C	[49]
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	8.606x10 <sup>-30</sup> C-m	[49],[10]
Ionization potential:	9.85 eV	[41]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	8.661 kJ/mol	[49]
Heat of vaporization:	47.6324 kJ/mol	[105]
	45.23	[49]
Heat of sublimation:	unknown	
Heat capacity @ 30°C:	0.2209 kJ/(mol-K) (liq)	[49]
Heat of combustion:	unknown	
Heat of formation:	unknown	
Gibbs (free) energy:	unknown	
<b>Analytical chemistry:</b>		
pP <sub>oct</sub> =	1.58	[8],[41]
	1.46	[31]
	1.29	[23]
	1.12	[27],[41]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	-2.18	[49]
Henry's law constant =	0.00132 kPa-m <sup>3</sup> /mol	[41]
Hydrolysis half-life =	1.6x10 <sup>7</sup> to 6.3x10 <sup>7</sup> sec	[8]
	6.3x10 <sup>8</sup> sec	[31]

**Electrochemical data:** Unknown

**Clay-organic interaction data:** Unknown

**Solubility:** Very slightly soluble in water. Soluble in ethanol, ether, acetone. Miscible with benzene, most organic solvents. [105],[22],[10]

1.02 wt% in water @ 20°C	[49],[104]
1.07 wt% in water @ 20°C	[10]
1.1 wt% in water @ 20°C	[32]

**Form:** Colorless liquid. Sweet, chloroform-like or ethylene dichloride-like odor or pungent, fruity odor. [51],[107],[22],[56],[108],[32]

## 152 - Bis(2-chloroethyl) ether

**Use:** General solvent for cellulose esters, naphthalenes, oils, fats, greases, pectin, tar, gum; selective solvent of producing high-grade lubricating oils; in textiles as a fulling compound and scouring and cleansing; wetting and penetrating compounds; organic synthesis; manufacture of paint, varnish, lacquer, finish remover, soap; manufacture of butadiene, medicinals, pharmaceuticals; dry cleaning; soil fumigant; lead scavenger during production of gasoline anti-knock compounds. [22],[56],[104],[32]

**Fire and explosion hazard:** Moderate.

Flash point: (CC) 55°C [51],[107],[22],[49],[32]

(CC) 63°C [108]

(OC) 82.2°C [107]

(OC) 85°C [49]

uel: unknown

lel: unknown

Autoign. temp.: 369°C [51],[107],[22],[32]

Flammable liquid. Moderate fire hazard when exposed to heat, flame, or oxidants. Reacts vigorously with oleum, chlorosulfonic acid. Emits highly toxic fumes of phosgene, carbon monoxide and hydrogen chloride when heated to decomposition. May react with water or steam to evolve toxic and corrosive fumes. Fight fire with alcohol or polymer foam, dry chemical powder, CO<sub>2</sub>. [51],[107],[32],[55]

**Incompatibility:** Oleum; chlorosulfonic acid; oxidizing materials. [51],[56],[32]

**Handling:** Keep away from heat, flame, and sources of ignition. Do not inhale mist or vapor (appropriate respirator or self-contained breathing apparatus required). Prevent skin or eye contact (nitrile, PVA, or rubber gloves and lab coat; splash-proof chemical goggles). Readily absorbed through skin. Facilities for eye wash and quick body drenching should be available. Contaminated clothing should be removed and cleaned. Use with adequate ventilation (fume hood). Keep container tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet. Store in glass bottles in secure poison area. [22],[56],[53],[32],[55]

**Health effects:** DCEE is a poison and potential human carcinogen. Routes of entry are inhalation of vapor, percutaneous absorption, ingestion, and eye and skin contact. Points of attack include respiratory system, skin and eyes, liver, and kidneys. Vapor or mist is irritating to the mucous membranes of the eyes, nose, and upper respiratory tract causing profuse lacrimation, coughing and nausea. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. Liquid causes mild irritation of the skin. May cause first-degree skin burns on short exposure. Ingestion causes irritation of the mouth and stomach with symptoms of systemic poisoning. Mild bronchitis may result from repeated exposure to low concentrations. It is a mild narcotic. Chronic overexposure may result in carcinogenic effects. [51],[107],[56],[32],[55]



**Toxicity:** High.

TWA: 5 ppm (30 mg/m<sup>3</sup>) (skin) [1]

STEL: 10 ppm (60 mg/m<sup>3</sup>) (skin) [1]

CL: 15 ppm (90 mg/m<sup>3</sup>) (skin) [51]

IDLH: 250 ppm (1460 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 35 ppm (200 mg/m<sup>3</sup>) [51]

<15 ppm (90 mg/m<sup>3</sup>) [104]

15 ppm (90 mg/m<sup>3</sup>) [32]

Carcinogenicity: possible human carcinogen [56],[107]

positive results in some animals [56],[107],[55]

Mutagenicity: unknown

**Exposure:**

**External:**

Non-lethal: 3 ppm (18 mg/m<sup>3</sup>) -- eye irritation [56]

35 ppm (200 mg/m<sup>3</sup>) -- practically free from irritation[104]

260 ppm (1520 mg/m<sup>3</sup>) -- eye irritation [51]

500-1000 ppm -- severe eye and nose irritation [51]

550 ppm -- intolerable eye and nose irritation [32]

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: unknown

**Inhalation:**

Short-term Inhalation Limits: 35 ppm (200 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: 100-260 ppm -- slight nausea and irritation [51]

Lethal: unknown

## 154 - Bis(chloromethyl) ether

Bis(chloromethyl) ether

 $C_2H_4Cl_2O$ 

CAS RN: 542-88-1

Syn: Bis(chloromethyl) ether \* Methane, oxybis[chloro- \* BCME \*  
 Chloro(chloromethoxy) methane \* Chloromethyl ether \* Dichlorodimethylether  
 \*  $\alpha,\alpha'$ -Dichlorodimethyl ether \* sym-Dichloro-dimethyl ether \* sym-  
 Dichloromethyl ether \* Dichloromethyl ether \* Dimethyl-1,1'-dichloroether \*  
 Monochloromethyl ether \* Oxybis(chloromethane) \*

Molecular formula:  $ClCH_2-O-CH_2Cl$ 

Polychlorinated Aliphatic Ether

## Physical properties:

Relative molecular mass:	114.959	
Specific gravity:	1.315	[51], [104], [108]
	1.328 (15/4)	[105], [10]
	1.323 (15/4)	[106]
Boiling point:	106.°C	[23]
	105.°C	[51]
	104.°-105°C	[10]
	104.°C	[105], [104], [106]
Melting point:	-41.5°C	[105], [104], [106]
Refractive index:	1.435 @ 21°C	[105], [106]
	1.4346	[108]
Vapor pressure:	4.0 kPa @ 22°C (30mm)	[23]
Vapor density:	4.0	[51]
	3.97	[104]

Evaporation rate:	unknown
Relative dielectric permittivity:	unknown
Loss tangent:	unknown
Relaxation time:	unknown
Thermal conductivity:	unknown
Electrical resistivity:	unknown
Critical temperature:	unknown
Critical pressure:	unknown
Dynamic viscosity:	unknown
Kinematic viscosity:	unknown
Surface tension:	unknown
Contact angle:	unknown
Thermal expansion coefficient:	unknown
Compressibility:	unknown
Vapor diffusivity:	unknown
Solution diffusivity:	unknown
Electric dipole moment:	unknown
Ionization potential:	unknown
Magnetic volume susceptibility:	unknown
Speed of sound:	unknown
Heat of melting:	unknown
Heat of vaporization:	unknown
Heat of sublimation:	unknown
Heat capacity @ 25°C:	unknown
Heat of combustion:	unknown
Heat of formation:	unknown
Gibbs (free) energy:	unknown

Analytical chemistry:  $pP_{oct}$  = -0.38 [8],[31]  
 $pK_s$  = unknown  
 $pK_a$  = NA [31]  
 $pK_{BH}$  = unknown  
Henry's law constant =  
Hydrolysis half-life =  $2.5 \times 10^1$  sec [13]  
 $3.8 \times 10^1$  sec [8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Decomposes in water. Miscible with ethanol, ether. [105]  
2.2 wt% in water (calculated) [8]

Form: Volatile, colorless liquid. Suffocating odor. [51],[5]

Use: Intermediate for ion-exchange resins; laboratory reagent; manufacture of polymers. [22],[5]

Fire and explosion hazard: Very high.

Flash point:  $< -7.2^\circ\text{C}$  [51]

uel: unknown

lel: unknown

Autoign. temp.: unknown

Extremely flammable liquid. Emits very toxic fumes of  $\text{Cl}^-$  when heated to decomposition. [51]

Incompatibility: Unstable in moist air. Rapidly hydrolyzes in water into hydrogen chloride and formaldehyde. [108],[23]

Handling: WARNING: avoid all contact. Keep away from heat, sparks, sources of ignition. This substance is carcinogenic and all contact with liquid or vapor should be prevented. Do not breathe vapor (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (chemical resistant gloves and suit; safety goggles or face shield). Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [1]

Health effects: BCME is a poison and a confirmed human carcinogen. Routes of entry are inhalation, ingestion, and eye and skin contact. Points of attack include respiratory system, eyes, and skin. It can cause skin and eye damage and is believed to cause lung cancer. It is a strong irritant to eyes and respiratory tract. [1],[5],[108]

156 - *Bis(chloromethyl) ether*

**Toxicity:** Very high.

TWA: 0.001 ppm (0.005 mg/m<sup>3</sup>) -- confirmed human carcinogen [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: confirmed human carcinogen, all isomers; lung-cancer  
[1],[51],[22],[104]

most potent carcinogen [103]

Mutagenicity: an experimental mutagen [51]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: 100 ppm (470 mg/m<sup>3</sup>) for 3 min [51]

Bis(2-ethylhexyl) phthalate

C<sub>24</sub>H<sub>38</sub>O<sub>4</sub>

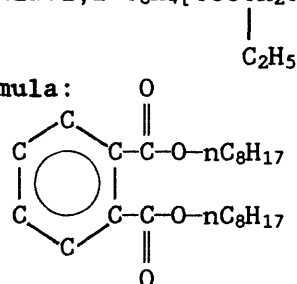
CAS RN: 117-81-7

Syn: Bis(2-ethylhexyl) phthalate \* 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester \* BEHP \* bis(2-ethylhexyl)-1,2-benzenedicarboxylate \* Bis(2-ethylhexyl) ester phthalic acid \* Bisoflex 81 \* Bisoflex DOP \* Compound 889 \* DAF 68 \* DEHP \* Di(ethylhexyl) phthalate \* Di(2-ethylhexyl) phthalate \* Di(2-ethylhexyl) ortho-phthalate \* Dioctyl phthalate \* Di-sec-octyl phthalate \* DOP \* Ergoplast FDO \* Ethylhexyl phthalate \* 2-Ethylhexyl phthalate \* Eviplast 80 \* Eviplast 81 \* Fleximel \* Flexol DOP \* Flexol plasticizer DOP \* Good-rite GP 264 \* Hatcol DOP \* Hercoflex 260 \* Kodaflex DOP \* Mollan O \* NCI-C52733 \* Nuoplaz DOP \* Octoil \* Octyl phthalate \* Palatinol AH \* Phthalic acid, bis(2-ethylhexyl) ester \* Phthalic acid, dioctyl ester \* Pittsburgh PX-138 \* Platinol AH \* Platinol DOP \* RC plasticizer DOP \* RCRA Waste Number U028 \* Reomol DOP \* Reomol D 79P \* Sicol 150 \* Staflex DOP \* Truflex DOP \* Vestinol AH \* Vinicizer 80 \* Witcizer 312 \*

Molecular formula: 1,2-C<sub>6</sub>H<sub>4</sub>[COOCH<sub>2</sub>CHCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>]<sub>2</sub>

Dicarboxylic Acid Ester

Structural formula:

**Physical properties:**

Relative molecular mass:	390.563	
Specific gravity:	0.9843	[10], [49]
Boiling point:	387.°C	[56]
	385.°C	[104]
	384.°C	[10], [49]
Melting point:	-50.°C	[10], [49]
	-55.°C	[104]
Refractive index:	1.4859	[10], [49]
	1.4836	[22]
Vapor pressure:	2.6x10 <sup>-8</sup> kPa @ 20°C (2x10 <sup>-7</sup> mm)	[41]
	8.3x10 <sup>-9</sup> kPa @ 25°C (6.2x10 <sup>-8</sup> mm)	[41]
	6.6x10 <sup>-9</sup> kPa @ 68°C (5x10 <sup>-8</sup> mm)	[41]
	0.07 @ 183°C (0.5 mm)	[49]
	0.160 @ 200°C (1.2mm)	[104]
	0.176 @ 200°C (1.32mm)	[22]
	0.7 @ 231°C (5mm)	[49]
Vapor density:	13.45	[104]
	>16.	[55]
Evaporation rate:	unknown	
Relative dielectric permittivity:	5.3 @ 20°C	[10], [49]
	5.1 @ 25°C	[11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	

# 158 - Bis(2-ethylhexyl) phthalate

Critical pressure:	unknown	
Dynamic viscosity:	381. mPa-s @ 0°C	[49]
	81.4 @ 20°C	[10],[22]
	56.5 @ 25°C	[49]
Kinematic viscosity:	387. $\mu\text{m}^2/\text{s}$ @ 0°C	
	82.7 @ 20°C	
	57.4 @ 25°C	
Surface tension:	15. mN/m @ 20°C	[107]
Contact angle:	unknown	
Thermal expansion coefficient:	0.00076 K <sup>-1</sup> @ 20°C	[49]
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	9.473x10 <sup>-30</sup> C-m @ 20°C	[10],[49]
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	unknown	
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	unknown	
Heat of combustion:	-13747. kJ/mol @ 25°C (liq)	[107]
Heat of formation:	unknown	
Gibbs (free) energy:	unknown	
Analytical chemistry: pP <sub>oct</sub> =		
	9.61	[31]
	8.73	[8]
	5.3	[8]
	5.11	[23]
	4.2	[41]
	pK <sub>s</sub> = NA	
	pK <sub>a</sub> = NA	[31]
	pK <sub>BH</sub> = NA	
Henry's law constant =	0.00111 kPa-m <sup>3</sup> /mol @ 25°C (calc)	[41]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water. Miscible with mineral oil, hexane. [22],[104],[41]

0.00004 wt% in water @ 25°C	[41]
<0.01 wt% in water @ 20°C	[107],[49]
0.0000285 wt% technical grade in water @ 24°C	[104]

Form: Colorless to light-colored oily liquid. Mild odor. [107],[22]

Use: Plasticizer for many resins and elastomers; organic pump fluid; plastics manufacturing, processing, and recycling. [22],[56],[104]

**Fire and explosion hazard:** Low.

Flash point: (OC) 218°C [107],[22],[49]

UEL: unknown

LEL: 0.3% [55]

Autoign. temp.: 390°C [55]

Combustible liquid. Emits acrid smoke, CO and CO<sub>2</sub> when heated to decomposition. Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder. Foam and water spray are effective but may cause frothing. [51],[107],[55]

**Incompatibility:** Nitrates; strong oxidizers; strong acids; strong alkalines. [107],[56]

**Handling:** Do not breathe vapor or mist (appropriate respirator or self-contained breathing apparatus. Do not get in eyes, on skin, or on clothing (resistant gloves, safety goggles, other protective clothing). Use in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in cool, dry, well-ventilated area. [56],[55]

**Health effects:** DOP is a mild irritant. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include eyes, upper respiratory system, gastrointestinal system. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Symptoms of exposure include skin irritation, nausea and diarrhea. Chronic overexposure may have carcinogenic effects. Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. [56],[51],[55]

**Toxicity:** Very low.

TWA: 0.3 ppm (5 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: possible human carcinogen [1],[51]

proven animal carcinogen [56],[26]

Mutagenicity: possible human mutagen [51]

possible teratogen [55]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: 143 mg/kg body wt -- gastrointestinal effects, diarrhea, constipation, ulceration [51]

Lethal: unknown

Inhalation:

Non-lethal: unknown

Lethal: unknown

## 160 - Bromoform

Bromoform

CHBr<sub>3</sub>

CAS RN: 75-25-2

Syn: Bromoform \* Methane, tribromo- \* Methenyl tribromide \* Methyl tribromide \* NCI-C55130 \* RCRA Waste Number U225 \* Tribromomethane \* UN 2515 (DOT) \*

Molecular formula: CHBr<sub>3</sub>

Polybrominated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	252.731	
Specific gravity:	2.8909	[49]
	2.890	[51], [104], [48]
	2.8899	[105]
	2.887	[22]
	2.85	[32]
Boiling point:	151.2°C	[22]
	150.°C	[48]
	149.6°C	[10]
	149.5°C	[56], [105]
	149.21°C	[49]
	149.°C	[104]
	148.°C	[32]
Melting point:	9.°C	[22]
	8.3°C	[105]
	8.1°C	[10]
	8.05°C	[49]
	7.9°C	[48]
	7.8°C	[32]
	6.°-7°C	[51], [56], [104]
Refractive index:	1.59763	[49]
	1.5976	[105]
	1.6005 @ 15°C	[10], [22]
Vapor pressure:	0.667 kPa @ 20°C (5mm)	[3], [32]
	0.7466 @ 25°C (5.6mm)	[104]
	0.79 @ 25°C (5.9mm)	[49]
	1.33322 @ 34°C (10mm)	[105]
Vapor density:	8.7	[104], [32]
Evaporation rate:	unknown	
Relative dielectric permittivity:	4.404 @ 10°C	[2]
	4.39 @ 20°C	[49], [10], [105], [11]
	4.385 @ 20°C	[2]
	4.5 @ 20°C	[22]
	4.39 @ 25°C	[2]
	4.38 @ 25°C	[2]
	3.816 @ 40°C	[2]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	>0.5 MOhm-m @ 25°C	[49], [11], [10]
Critical temperature:	unknown	
Critical pressure:	unknown	



Dynamic viscosity:	2.151 mPa-s @ 15°C	[49]
	2.152 @ 15°C	[10], [48]
	1.89 @ 25°C	[105]
	1.741 @ 30°C	[49], [48]
Kinematic viscosity:	0.745 $\mu\text{m}^2/\text{s}$ @ 15°C	
	0.654 @ 25°C	
	0.602 @ 30°C	
Surface tension:	46.83 mN/m @ 10°C vapor	[10]
([10] values are calculated)	45.52 @ 20°C	[10]
	41.53 @ 20°C vapor	[105], [22]
	45.10 @ 24.8°C	[49]
	44.22 @ 30°C	[10]
	42.91 @ 40°C	[10]
	42.30 @ 41.7°C	[49]
	41.60 @ 50°C	[10]
	40.29 @ 60°C	[10]
	38.98 @ 70°C	[10]
	37.68 @ 80°C	[10]
	36.37 @ 90°C	[10]
	35.06 @ 100°C	[10]
Contact angle:	unknown	
Thermal expansion coefficient:	0.00091 K <sup>-1</sup> @ 20°C	[48]
Compressibility:	unknown	
Vapor diffusivity:	2.9 $\mu\text{m}^2/\text{s}$ in acetone	[47]
	0.53 in i-amylalcohol	[47]
	1.08 in ethanol	[47]
	3.62 in ethyl ether	[47]
	2.20 in methanol	[47]
	0.94 in n-propanol	[47]
Solution diffusivity:	unknown	
Electric dipole moment:	3.30x10 <sup>-30</sup> C-m	[49], [105]
Ionization potential:	10.51 eV (PI)	[105]
Magnetic volume susceptibility:	-11.9x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	38.91 kJ/mol	[49]
	40.50	[105]
Heat of sublimation:	unknown	
Heat capacity @ 17-21°C:	0.13284 kJ/(mol-K) (liq)	[49]
@ 20°C:	0.1355 (liq)	[48]
@ 25°C:	0.130 (liq)	[105]
	0.07101 (gas)	[10]
	0.0712 (gas)	[105]
Heat of combustion:	-440.03 kJ/mol @ 25°C (liq)	[20]
	-485.7 (gas)	[20]
Heat of formation:	-28.5 kJ/mol @ 25°C (liq)	[49], [105]
	16.736 (gas)	[49]
	16.747 (gas)	[10], [105]
Gibbs (free) energy:	7.453 kJ/mol @ 25°C (gas)	[10]

## 162 - Bromoform

Analytical chemistry:  $P_{oct}$  = 2.38 [31],[41]  
2.30 [8],[41]  
 $pK_s$  = unknown  
 $pK_a$  = 11.8 @ 20°C in water [52]  
 $pK_{BH}$  = unknown  
Henry's law constant = 0.0567 kPa·m<sup>3</sup>/mol [41]  
0.0539 [41]  
Hydrolysis half-life = 2.2x10<sup>10</sup> sec [13]  
2.1x10<sup>9</sup> [8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Slightly soluble in water. Soluble in solvent naphtha, fixed and volatile oils. Miscible with benzene, chloroform, ethanol, ether. [105],[22],[10],[32],[49],[108],[104]

0.1 wt% in water @ 20°C [32]  
0.1 wt% in cold water [10]  
0.318 wt% in water @ 30°C [49]  
0.00125 vol% in water [108]  
0.319 wt% in water @ 30°C [104]

Form: Colorless to yellow liquid or hexagonal crystals. Chloroform-like odor. Sweetish taste. Gradually decomposes acquiring a yellow color. Air and light accelerate the decomposition. Commercial preparations have 3-4% alcohol added as a preservative. [51],[107],[56],[22],[104],[32]

Use: Heavy liquid flotation agent in mineral separation-sedimentary petrographical surveys, geological assays, and purification of materials such as quartz; in chemical and pharmaceutical synthesis in condensation reactions; source of free radicals to initiate transformation of various compounds; industrial solvent in liquid-solvent extractions in nuclear magnetic resonance studies; flame retardant in compositions for cellulose and microencapsulation; catalyst, initiator, or sensitizer in polymer production, irradiation reactions and vulcanization of rubber; an ingredient in pharmaceuticals or medicinal products; solvent for waxes, greases and oils. [56],[22],[104],[32]

Fire and explosion hazard: Very low.

Flash point: (CC) <79°C [49]

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable liquid or solid. Emits highly toxic fumes of hydrogen bromide and bromine when heated to decomposition. Can be an explosion hazard, especially when heated. [51]

Incompatibility: Acetone; potassium hydroxide; chemically-active metals such as Na, K, Ca, Li, powdered aluminum, zinc and magnesium; strong bases (caustic alkalis). [51],[56]

**Handling:** Keep away from heat and light. Use with adequate ventilation (fume hood). Avoid breathing vapor (appropriate respirator or self-contained breathing apparatus). Prevent any reasonable probability of contact with eyes and skin (goggles and face shield; neoprene, natural rubber or latex gloves and overclothing). Remove non-impervious clothing promptly if wet or contaminated. Keep container tightly closed. Store in secure poison area. [56],[32]

**Health effects:** Bromoform is a poison, irritant, narcotic, hepatotoxin and suspected human carcinogen. Routes of entry are ingestion, inhalation, skin absorption, and eye and skin contact. Points of attack include skin, liver, kidneys, respiratory system, lungs, and central nervous system. Vapors or fluid can cause irritation of skin, eyes, and mucous membranes. Inhalation of vapors may cause lachrymation, coughing, chest pains, difficulty breathing or unconsciousness. Ingestion may also cause dizziness, disorientation and slurred speech, unconsciousness and death. Chronic effects of overexposure may include central nervous system depression, liver damage and death. Abuse may lead to habituation or addiction. It has anesthetic properties similar to those of chloroform. [51],[56],[32]

**Toxicity:** Moderate.

TWA: 0.5 ppm (5 mg/m<sup>3</sup>) (skin) [1]  
STEL: no value set [1]  
CL: unknown  
IDLH: no value set [56]  
Peak: unknown  
Odor threshold: 0.3-3 ppm (3-30 mg/m<sup>3</sup>) [104]  
Carcinogenicity: potential human carcinogen [56]  
Mutagenicity: unknown

**Exposure:** Unknown

## 164 - Bromomethane

Bromomethane

CH<sub>3</sub>Br

CAS RN: 74-83-9

Syn: Bromomethane \* Methane, bromo- \* Bercema \* Brom-o-gas \* Brom-o-gaz \* Curafume \* Dawson 100 \* Detia gas EX-M \* Dowfume \* Dowfume MC-2 \* Dowfume MC-33 \* Edco \* Embafume \* Fumigant-1 (obs.) \* Halon 1001 \* Haltox \* Iscobrome \* Kayafume \* MB \* M-B-C fumigant \* MBX \* MEBR \* Metafume \* Methogas \* Methyl bromide \* Monobromomethane \* Pestmaster (obs) \* Profume (obs.) \* R40B1 \* RCRA Waste Number U029 \* Rotox \* Terabol \* Terr-o-gas 67 \* Terr-o-gas 100 \* UN 1062 (DOT) \* Zytox \*

Molecular formula: CH<sub>3</sub>Br

Monobrominated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	94.9388	
Specific gravity:	1.7	[32]
	1.68	[107]
	1.6758	[49]
	1.6755	[105]
	1.732 (0/0)	[10], [51], [22]
	1.73 (0/0)	[104]
Boiling point:	4.6°C	[104]
	4.0°C	[48]
	3.6°C	[107], [32]
	3.56°C	[10], [105], [51], [108]
	3.55°C	[49]
	3.46°C	[22]
	3.°-4°C	[56]
Melting point:	-93.°C	[51], [107], [104], [48]
	-93.6°C	[105]
	-93.66°C	[108]
	-93.7°C	[10]
	-94.°C	[22], [32]
	-94.07°C	[49]
Refractive index:	1.4234	[10]
	1.4218	[105]
	1.4164	[49]
Vapor pressure:	53.33 kPa @ -11.9°C (400mm)	[105]
	166.6 @ 20°C (1250mm)	[22]
	185.4 @ 20°C (1391mm)	[32]
	202.65 @ 23°C (1520mm)	[105]
	217.7 @ 25°C (1633mm)	[49], [23]
	243.18 @ 25°C (1824mm)	[51]
	506.62 @ 54.8°C (3800mm)	[105]
Vapor density:	3.3	[107], [32]
	3.27	[51], [104]
Evaporation rate:	>1.	[32]
Relative dielectric permittivity:	10.91 @ -20°C	[49]
	9.82 @ 0°C	[105], [11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	NA	
Electrical resistivity:	NA	
Critical temperature:	194.°C	[105], [108]
	191.°C	[10], [49], [107]

Critical pressure:	8.451 MPa	[105]
Dynamic viscosity:	0.2174 mPa-s @ 0°C	[15]
	0.109 @ 15°C	[48]
	0.092 @ 30°C	[48]
Kinematic viscosity:	0.126 $\mu\text{m}^2/\text{s}$ @ 0°C	
	0.065 @ 15°C	
	0.055 @ 30°C	
Surface tension:	24.5 mN/m @ 15°C	[107]
Contact angle:	NA	
Thermal expansion coefficient:	NA	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	3.3023x10 <sup>-30</sup> C-m	[105]
	5.77x10 <sup>-30</sup>	[49]
Ionization potential:	10.53 eV (S,PI)	[105]
Magnetic volume susceptibility:	-13.12x10 <sup>-6</sup> SI units @ 0°C	[105]
Speed of sound:	unknown	
Heat of melting:	5.983 kJ/mol	[10], [107]
	5.978	[105]
Heat of vaporization:	24.8106 kJ/mol	[105]
	24.098	[49]
	23.9276	[10]
	23.738	[107]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.11707 kJ/(mol-K) (liq)	[49]
	0.04250 (gas)	[10], [105]
Heat of combustion:	-763.6 kJ/mol @ 25°C (liq)	[49]
	-787.0 (gas)	[49]
	-770.37 @ 20°C (gas)	[105]
Heat of formation:	-61.0 kJ/mol @ 25°C (liq)	[49]
	-37.76 (gas)	[10]
	-37.74 (gas)	[49]
	-35.17 (gas)	[105]
Gibbs (free) energy:	-28.26 (gas)	[10]
	-26.0 (gas)	[105]
Analytical chemistry: pP <sub>oct</sub> =	1.19	[23], [21]
	1.1	[8], [41]
	1.09	[31]
	1.00	[41]
	pK <sub>s</sub> = unknown	
	pK <sub>a</sub> = NA	[31]
	pK <sub>BH</sub> = unknown	
Henry's law constant =	20.3 kPa-m <sup>3</sup> /mol	[41]
	3.04	[41]
Hydrolysis half-life =	1.7x10 <sup>6</sup> sec	[13], [8]

Electrochemical data: Meites and Zuman (1977).

Clay-organic interaction data: Unknown

## 166 - Bromomethane

**Solubility:** Very slightly soluble in water. Miscible with ethanol, acetone, chloroform, carbon disulfide, carbon tetrachloride, benzene, ether, n-heptane, most organic solvents. [105],[22],[15],[10],[108]

0.09 wt% in water @ 20°C [104]  
<0.1 wt% in water @ 20°C [32]

**Form:** Colorless, transparent, volatile liquid or gas. Odorless to sweet, chloroform-like odor at high concentrations. Burning taste. Shipped as a liquified gas. [51],[107],[56],[22],[104],[108]

**Use:** Primary use is as an insect fumigant for soil, grain, warehouses, mills, ships, etc. Disinfestation of potatoes, tomatoes, and other crops; food sterilization for, pest control in fruits, vegetables, dairy products, nuts, and grains; chemical intermediate and methylating agent in the manufacture of ammonium compounds and organo-tin derivatives; refrigerant; herbicide; fire extinguishing agent; low-boiling solvent in aniline dye manufacture; wool degreaser; extraction of oils from vegetable, nuts, seeds, and flowers; in ionization chambers. [56],[22],[104],[32],[108],[41]

**Fire and explosion hazard:** Low

Flash point: none [51],[22],[32]

uel: 15% [107]

14.5% [51]

lel: 10% [107]

13.5% [51]

Autoign. temp.: 537.7°C [107]

536.7°C [51]

Practically nonflammable, poisonous, corrosive liquid or gas. Forms explosive mixture in air within narrow explosion limits at atmospheric pressure, but wider limits at higher pressures. Low fire and explosion hazard when exposed to heat or flame. Emits highly toxic and irritating fumes of bromides, hydrogen bromide, CO, and CO<sub>2</sub> when heated to decomposition. Fight fire with dry chemical powder, alcohol or polymer foam, CO<sub>2</sub>. Do not extinguish burning gas if flow cannot be shut off immediately. Use water spray or fog nozzle to keep cylinder cool. [51],[107],[32],[55]

**Incompatibility:** Strong oxidizers; aluminum and its alloys; dimethyl sulfoxide, ethylene oxide; plastics; rubber. WARNING: metallic components of zinc, aluminum, and magnesium (or their alloys) are unsuitable for service with bromomethane because of the formation of pyrophoric grignard-type compounds. [51],[56],[32],[55]

**Handling:** Avoid heat, flame, and sources of ignition. Cylinder temperature should not exceed 52°C (125°F). Prevent inhalation of gas (appropriate respirator or self-contained breathing apparatus). Wear appropriate clothing to prevent any possibility of skin and eye contact (neoprene or PVA overclothing and gloves; chemical goggles). WARNING: methyl bromide readily penetrates rubber gloves; use gloves constructed from tetrafluoroethylene polymer. It may be absorbed by leather. Use only in a chemical fume hood. Remove non-impervious clothing promptly if wet or contaminated. Emergency showers should be provided. Keep container tightly closed. Store in cool, well-ventilated, secure poison area. [107],[56],[32],[55]

**Health effects:** Bromomethane is a poison and has narcotic effects. It is one of the most toxic of the common organic halide gases. Routes of entry are inhalation, percutaneous absorption, ingestion, skin and eye contact. Points of attack include the central nervous system, respiratory system, lungs, liver, kidneys, skin, and eyes. May be fatal if inhaled as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. It is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin and may produce severe burns. It is hematotoxic and narcotic with delayed action. Onset of symptoms may be delayed from 4-6 hours and up to 48 hours. Effects are cumulative and damaging to the nervous system (including brain damage), kidneys, and lungs. CNS effects include blurred speech, mental confusion, numbness, tremors, speech defects. In fatal poisonings, the early symptoms are headache, visual disturbance, nausea and vomiting, smarting of the eyes, skin irritation, listlessness, vertigo and tremor. Progress is nearly always rapid, with the development of convulsions, fever, pulmonary edema, cyanosis, unconsciousness, and death. Pulmonary symptoms are relatively slight. It is a possible carcinogen. [51],[107],[56],[32],[108],[55]

**Toxicity:** Low

TWA: 5 ppm (20 mg/m<sup>3</sup>) (skin) [1]  
 STEL: no value set [1]  
 CL: 20 ppm (75 mg/m<sup>3</sup>) (skin) [51],[56]  
 IDLH: 2000 ppm (750 mg/m<sup>3</sup>) [107],[56]  
 Peak: unknown  
 Odor threshold: relatively odorless [107]  
 Carcinogenicity: suspected or confirmed human carcinogen [1]  
 Mutagenicity: unknown

**Exposure:**

External:

Non-lethal: 40 g/m<sup>3</sup> for 40 min -- blistering of skin [110]  
 Lethal: unknown

Oral:

Non-lethal: unknown  
 Lethal: unknown

Inhalation:

Short-term Inhalation Limits: 20 ppm (75 mg/m<sup>3</sup>) for 5 min [107]  
 Non-lethal: 100-500 ppm (388-1940 mg/m<sup>3</sup>) [51]  
 Lethal: 8600-60000 ppm -- has always resulted in fatality [51]  
     60000 ppm (233 g/m<sup>3</sup>) for 2 hr -- death of an adult human [51]  
     1.3 ppm (5 mg/m<sup>3</sup>) for 2 hr -- death of a child [51]  
     26 ppm (1 g/m<sup>3</sup>) for 2 hr -- death of a child [55]

## 168 - 2-Butanone

2-Butanone

C<sub>4</sub>H<sub>8</sub>O

CAS RN: 78-93-3

Syn: 2-Butanone \* Butanone \* 3-Butanone \* Ethyl methyl ketone \* Meetco \*  
 MEK \* Methyl acetone \* Methyl ethyl ketone \* RCRA Waste Number U159 \* UN  
 1193 (DOT) \* UN 1232 (DOT) \*

Molecular formula: CH<sub>3</sub>COCH<sub>2</sub>CH<sub>3</sub>

Aliphatic Ketone

## Physical properties:

Relative molecular mass:	72.1069	
Specific gravity:	0.806	[107]
	0.8054	[105]
	0.805	[104], [22]
	0.8049	[10], [49]
Boiling point:	79.6°C	[105], [104], [10], [107]
	79.583°C	[49]
	79.57°C	[51]
	79.°-80°C	[56]
Melting point:	-85.9°C	[51]
	-86.3°C	[107]
	-86.35°C	[105]
	-86.4°C	[104]
	-86.69°C	[49]
	-86.7°C	[10]
Refractive index:	1.3788	[49], [105], [10]
	1.379	[22]
Vapor pressure:	1.333 kPa @ -17.7°C (10mm)	[105]
	5.333 @ 6°C (40mm)	[105]
	9.493 @ 20°C (71.2mm)	[51]
	10.333 @ 20°C (77.5mm)	[104]
	12.079 @ 25°C (90.60mm)	[49]
	13.332 @ 25°C (100mm)	[105]
Vapor density:	2.5	[107]
	2.42	[51]
	2.41	[104]
Evaporation rate:	3.8	[49]
Relative dielectric permittivity:	22.27 @ -20°C	[11]
	20.30 @ 0°C	[11]
	18.51 @ 20°C	[49], [105], [10], [11]
	17.71 @ 30°C	[49]
	16.81 @ 40°C	[11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	0.1 MOhm-m @ 25°C	[11], [10]
	2.78	[49]
Critical temperature:	263.63°C	[49]
	262.5°C	[107]
	262.4°C	[10]
	262.°C	[105]
Critical pressure:	4.207 MPa	[49]
	4.194	[10]
	4.15	[105], [107]



Dynamic viscosity:	0.423 mPa-s @ 15°C	[10]
	0.40 @ 20°C	[22]
Kinematic viscosity:	0.523 $\mu\text{m}^2/\text{s}$ @ 15°C	
	0.497 @ 20°C	
Surface tension:	26.9 mN/m @ 0°	[49]
	24.6 @ 20°C (air/vapor)	[49], [105]
	23.97 @ 24.8°C	[49]
Contact angle:	unknown	
Thermal expansion coefficient:	0.00119 K <sup>-1</sup>	[49]
Compressibility:	1.116x10 <sup>-6</sup> nPa <sup>-1</sup> @ 20°C	[49]
	1.188x10 <sup>-6</sup> @ 25°C	[49]
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	6.086x10 <sup>-30</sup> C-m	[10]
Ionization potential:	9.5 eV (PI)	[105]
Magnetic volume susceptibility:	-6.40x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	8.445 kJ/mol	[10]
	8.439	[49], [105]
Heat of vaporization:	31.296 kJ/mol	[10]
	31.8 @ bp	[49]
	32.017	[107]
	34.120	[105]
	34.51 @ 25°C	[49]
Heat of sublimation:	34.918 kJ/mol	[10]
Heat capacity @ 25°C:	0.1592 kJ/(mol-K) (liq)	[105]
	0.1590 (liq)	[10]
	0.15891 (liq)	[49]
	0.10295 (gas)	[10]
Heat of combustion:	-2445.8 kJ/mol @ 20°C (liq)	[105]
	-2438.44 @ 25°C (liq)	[49]
Heat of formation:	-273.34 kJ/mol @ 25°C (liq)	[10]
	-278.99 (liq)	[49]
	-235.55 (gas)	[10]
	-238.57 (gas)	[49]
Gibbs (free) energy:	-151.48 kJ/mol @ 25°C (liq)	[10]
	-146.16 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	0.29	[21], [24], [41]
	0.26	[104], [21], [41]
pK <sub>s</sub> =	25.94 @ 25°C	[49]
pK <sub>a</sub> =	14.7 @ 25°C	[49]
pK <sub>BH</sub> =	-7.2 in aq H <sub>2</sub> SO <sub>4</sub>	[49]
Henry's law constant =	0.00472 kPa-m <sup>3</sup> /mol @ 25°C	[41]
	0.00106	[24]
Hydrolysis half-life =	unknown	

Electrochemical data: Meites and Zuman (1977), Feoktistov (1983)

Clay-organic interaction data: Unknown

## 170 - 2-Butanone

**Solubility:** Soluble in water. Miscible with ethanol, ether, acetone, benzene, oils. [105],[22],[10],[49],[104]

35.3 wt% in water @ 10°C	[104]
24.0 wt% in water @ 20°C	[49]
22.6 wt% in water	[22]
25.5 wt% in water @ 25°C	[41]
24.1 wt% in water @ 30°C	[41]
19.0 wt% in water @ 90°C	[104]

**Form:** Clear, colorless liquid. Moderately pungent, neutral to unpleasant, acetone-like or mint-like odor. Commercial grades are 99.5% pure. [107],[51],[56],[22],[104]

**Use:** Solvent in nitrocellulose coatings and vinyl films; solvent or swelling agent of resins; intermediate in manufacture of ketones and amines; flush-off paint stripper; extraction and production of lubricating oil fractions of petroleum; smokeless powder manufacture; in cements and adhesives; dewaxing of lubricating oils; intermediate in drug manufacture; cleaning fluids; printing catalyst and carrier. Present in cigarette smoke (500 ppm) and gasoline exhaust (<1 ppm). [104],[56],[22]

**Fire and explosion hazard:** Very high.

Flash point: (CC) -6.667°C [107]  
(CC) -2°C [49]  
(OC) -5.556°C [107],[51]  
(OC) 1°C [49]

UEL: 11.5% [107],[51]

LEL: 1.8% [107],[51]

Autoign. temp.: 516.1°C [107]  
515.6°C [51]

Extremely flammable liquid. Dangerous fire hazard when exposed to heat or flame. Moderate explosion hazard when exposed to flame. Flash back along vapor trail may occur. Vapor may explode if ignited in an enclosed area. Fight fire with alcohol or polymer foam, dry chemical powder, CO<sub>2</sub>. Water may be ineffective. Cool exposed containers with water. [51],[107],[55]

**Incompatibility:** Very strong oxidizers; chlorosulfonic acid; oleum; potassium-tert-butoxide; heat or flame; chloroform; hydrogen peroxide, nitric acid; strong reducing agents. [51],[56],[55]

**Handling:** Avoid heat, flame, sparks, and sources of ignition. Prevent inhalation of vapor or mist (appropriate respirator or self-contained breathing apparatus). Wear appropriate clothing to prevent repeated or prolonged contact with liquid or vapor (neoprene or natural rubber or latex overclothes and gloves; chemical goggles). Remove non-impervious clothing promptly if wet or contaminated. Safety shower and eye bath should be provided. Keep container tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet. Store in secure poison area. [107]

**Health effects:** 2-Butanone is a poison. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include central nervous system, skin, and lungs. A strong irritant in high concentrations. High concentrations may cause temporary irritation of irritating to mucous membranes and upper respiratory tract. Prolonged exposure may cause nausea, vomiting, headache, dizziness, difficult breathing, loss of consciousness, gastrointestinal disturbances, dermatitis, or narcotic effect. Contact of the liquid with skin may cause smarting and reddening; will burn eyes. Harmful if swallowed. No permanent ill effects. [51],[107],[56],[55],[82]

**Toxicity:** Moderate.

TWA: 200 ppm (590 mg/m<sup>3</sup>) [1]

STEL: 300 ppm (885 mg/m<sup>3</sup>) [1]

CL: unknown

IDLH: 3000 ppm (8850 mg/m<sup>3</sup>) [56]

Peak: unknown

Odor threshold: 10 ppm (30 mg/m<sup>3</sup>) [107]

10-27 ppm (32-80 mg/m<sup>3</sup>) [104]

Carcinogenicity: unknown

Mutagenicity: experimental teratogen [51]

no genotoxicity found [44]

**Exposure:**

**External:**

Non-lethal: 350 ppm (1030 mg/m<sup>3</sup>) -- eye irritation [51]

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: unknown

**Inhalation:**

Short-term Inhalation Limits: 100 ppm (290 mg/m<sup>3</sup>) for 60 min [107]

Non-lethal: 100 ppm (295 mg/m<sup>3</sup>) for 5 min -- irritation [51]

>300 ppm (885 mg/m<sup>3</sup>) -- complaints [104]

700 ppm (2065 mg/m<sup>3</sup>) -- no permanent ill effects noted [104]

Lethal: unknown

## 172 - Cadmium

Cadmium

Cd

CAS RN: 7440-43-9

Syn: Cadmium \* Cd \* C.I. 77180 \* colloidal cadmium \*

Molecular formula: Cd

Element

## Physical properties:

Relative molecular mass:	112.41 ± 0.01	[105]
Specific gravity:	8.65	[47], [105]
	8.642	[22], [32], [105], [51], [22], [10]
	8.640	[48]
Boiling point:	770.°C	[10]
	767.° ± 2°C	[51], [48], [22]
	767.°C	[32]
	765.°C	[47], [105]
Melting point:	321.°C	[32]
	320.9°C	[47], [105], [51], [48], [22], [10]
Refractive index:	1.13 (sol)	[22], [105]
	0.82 (liq)	[105]
Vapor pressure:	essentially 0. kPa @ 20°C (0mm)	[32]
	0.1333 @ 394°C (1mm)	[47], [51]
	0.1333 @ 393°C (1mm)	[105]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	NA	
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	93.040 W/(m-K) @ 0°C	[48]
	92.65 @ 0°C	[10]
	93. @ 25°C	[105]
	91.877 @ 100°C	[48]
	85.62 @ 100°C	[10]
Electrical resistivity:	6.83x10 <sup>-14</sup> MOhm-m @ 0°C	[105]
	7.3x10 <sup>-14</sup> @ 22°C	[105]
	6.67x10 <sup>-14</sup>	[45]
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	630. mN/m @ 320°C	[20]
Contact angle:	NA	
Thermal expansion coefficient:	0.000030 K <sup>-1</sup> @ 25°C	[105], [48]
	0.000019 @ 100°C	[48]
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	5.0x10 <sup>16</sup> nm <sup>2</sup> /s @ 570°C in CdTe	[28]
Electric dipole moment:	NA	
Ionization potential:	8.991 eV (VUS)	[105]
Magnetic volume susceptibility:	-19.8x10 <sup>-6</sup> SI units (sol)	[105]
	-18.0x10 <sup>-6</sup> (liq)	[105]
Speed of sound:	unknown	
Heat of melting:	6.1183 kJ/mol	[48]
	6.113	[105]
	6.071	[10]

Heat of vaporization:	112.953 kJ/mol	[48]
	99.94	[10]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.0259 kJ/(mol-K) (sol)	[105]
	0.0260 (γ-sol)	[10]
	0.0208 (gas)	[10]
Heat of combustion:	unknown	
Heat of formation:	0.0 kJ/mol @ 25°C (γ-sol)	[10],[105]
	-0.59 (α-sol)	[10]
	112.9 (gas)	[105]
	112.1 (gas)	[10]
Gibbs (free) energy:	0.0 kJ/mol @ 25°C (γ-sol)	[10],[105]
	-0.59 (α-sol)	[10]
	78.25 (gas)	[105]
	77.50 (gas)	[10]
Analytical chemistry:	pP <sub>oct</sub> =	NA
	pK <sub>s</sub> =	NA
	pK <sub>a</sub> =	NA
	pK <sub>BH</sub> =	NA
	Henry's law constant =	NA
	Hydrolysis half-life =	NA

Electrochemical data: Hampson and Latham (1973)

Clay-organic interaction data: inorganic

Solubility: Insoluble in water. Soluble in acids. HNO<sub>3</sub>, NH<sub>4</sub>NO<sub>2</sub>, hot H<sub>2</sub>SO<sub>4</sub>. No reaction in alkalis. [32],[47],[105],[22],[10]

Form: Soft, bluish-white or silver-white, malleable metal easily cut by a knife (Mohs hardness of 2), with close-packed hexagonal structure. Available in the form of bars, sheets or wire, or a gray, granular powder. Odorless. It has atomic number 48 (Group IIB) and valence of 2. Major compounds include cadmium acetate, cadmium bromide, cadmium chloride, cadmium fluoroborate, cadmium nitrate, cadmium oxide, cadmium sulfate, and cadmium sulfide. It is slowly oxidized by moist air to form CdO. [105],[51],[54],[56],[10],[32],[108]

Use: It is a component of some of the lowest melting alloys. Cd and Cd compounds are used in bearing alloys with low coefficients of friction and great resistance to fatigue, extensively in electroplating (60% of use), in many types of solder, as depolarizers in silver-zinc storage batteries, in nickel-cadmium batteries, in rubber to improve heat resistance, in plastics to improve high-temperature properties, in paint pigments, in semiconductors for the conversion of solar energy to electrical power, as a barrier to control atomic fission, in photography and lithography, in fire protection systems, in selenium rectifiers, in black and white television phosphors, and in blue and green phosphors for color TV tubes. Cd compounds are also used as fungicides, insecticides, nematocides, polymerization catalysts, and in glass. It forms several salts, of which cadmium sulfate is the most common. [105],[54],[56],[22],[5]

## 174 - Cadmium

**Fire and explosion hazard:** Low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable solid. Moderate fire hazard in the form of dust when exposed to heat or flame or by chemical reaction with oxidizing agents, metals,  $\text{HN}_3$ , Zn, Se, and Te. Moderate explosion hazard in the form of dust when exposed to flame. Fight fire with  $\text{CO}_2$ , dry chemical powder. [51],[55]

**Incompatibility:** Oxidizing agents; metals; ammonia; potassium; zinc; selenium; sulfur; tellurium; acids; hydrazoic acid; ammonium nitrate. [51],[56],[55]

**Handling:** WARNING: avoid all contact. Avoid heat, flame, sparks or sources of ignition if dust or fumes are concentrated in the air. Prevent any reasonable possibility of inhalation, ingestion, or contact with skin, eyes, or clothing (appropriate respirator; rubber or leather gloves and overclothes; chemical goggles). Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [55],[56],[57]

**Health effects:** Cadmium and solutions of its compounds are highly toxic. Cd is a suspected human carcinogen, and several of the compounds are carcinogenic to animals. Routes of entry are inhalation of dust or fumes and ingestion. Points of attack include respiratory system, kidneys, liver, blood, prostate, and pancreas. When Cd or Cd compounds are ingested, the irritant and emetic action is so violent that little of the Cd is absorbed and fatal poisoning does not as rule ensue. Symptoms begin almost immediately after ingestion and may include sudden nausea, salivation, vomiting and diarrhea, and abdominal pain and discomfort. Inhalation of dust or fumes may cause dryness of the throat, cough, headache, a sense of constriction in the chest, dyspnea (shortness of breath), and vomiting. More severe exposures result in lung damage, with persistent cough, pain in the chest, severe dyspnea and prostration which may terminate in death. Symptoms may take several hours to appear so that fatal concentrations may be breathed without sufficient discomfort to warn a person. Cd is a common air and food contaminant. [105],[51],[54],[56],[108],[5],[63]

**Toxicity:** High.TWA: 0.002 ppm (10  $\mu\text{g}/\text{m}^3$ ) -- suspected human carcinogen [1]

STEL: no value set [1]

CL: 0.04 ppm (200  $\mu\text{g}/\text{m}^3$ ) in any 15 min period [51]

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: experimental and suspected human; animal positive.

[1],[51],[54],[56],[108]

animal sufficient evidence (IARC cancer review) [55]

carcinogenic by RTECS criteria [55]

Mutagenicity: experimental neoplastic effects, teratogen [51],[54]

equivocal tumorigenic agent by RTECS criteria [55]

**Exposure:**

## External:

Non-lethal: unknown

Lethal: unknown

## Oral:

Non-lethal: unknown

Lethal: 15 mg/kg body wt -- death of an adult male [51]

## Inhalation:

Short-term Inhalation Limit: unknown

Non-lethal: 0.02 ppm (88  $\mu\text{g}/\text{m}^3$ ) for 8.6 yrs -- systemic effects [51]Lethal: 8.5 ppm (39  $\text{mg}/\text{m}^3$ ) for 20 min -- death of an adult male [51]

# 176 - Carbon disulfide

Carbon disulfide

CS<sub>2</sub>

CAS RN: 75-15-0

Syn: Carbon disulfide \* Carbon bisulfide \* Carbon bisulphide \* Carbon disulphide \* Carbon sulfide \* Dithiocarbonic anhydride \* NCI-C04591 \* RCRA Waste Number P022 \* Sulphocarbonic anhydride \* UN 1131 (DOT) \* Weeviltox \*

Molecular formula: S=C=S

Inorganic Sulfide

## Physical properties:

Relative molecular mass:	76.131	
Specific gravity:	1.27	[32]
	1.2632	[105], [108], [106]
	1.26311	[49]
	1.263	[104], [48]
	1.2628	[10]
	1.26	[107]
Boiling point:	46.5°C	[51], [108]
	46.3°C	[107], [104], [48], [22], [32]
	46.26°C	[10]
	46.25°C	[105]
	46.225°C	[49]
	46.2°C	[106]
	46.°C	[56]
Melting point:	-108.6°C	[104]
	-110.8°C	[51]
	-111.°C	[22]
	-111.5°C	[106], [32]
	-111.53°C	[105]
	-111.57°C	[49]
	-111.6°C	[10], [107], [104], [108]
	-112.°C	[48]
Refractive index:	1.6319	[105], [106]
	1.62803	[108]
	1.6295	[10]
	1.62746	[49]
Vapor pressure:	1.05 kPa @ -10°C	(78.8mm) [41]
	13.3322 @ -5.1°C	(100mm) [105]
	1.697 @ 0°C	(127.3mm) [41]
	26.664 @ 10°C	(200mm) [104]
	34.664 @ 20°C	(260mm) [104]
	40.00 @ 20°C	(300mm) [32]
	48.21 @ 25°C	(361.6mm) [49]
	53.33 @ 28°C	(400mm) [105], [51]
	57.328 @ 30°C	(430mm) [104]
Vapor density:	2.67	[108]
	2.64	[51], [104]
	2.63	[10]
	2.6	[107], [32]
Evaporation rate:	22.6	[32]



Relative dielectric permittivity:	2.617 @ 0.5°C	[2]
	2.610 @ 11.5°C	[2]
	2.604 @ 14.6°C	[2]
	2.578 @ 18°C	[2]
	2.691 @ 18.3°C	[2]
	2.65 @ 19°C	[2]
	2.643 @ 20°C	[49]
	2.641 @ 20°C	[10],[105],[108]
	2.64 @ 20°C	[11],[2]
	2.579 @ 20°C	[2]
	2.590 @ 21.5°C	[2]
	2.58 @ 25°C (1 MHz)	[2]
	2.619 @ 30°C	[2]
	2.573 @ 30°C	[2]
	2.19 @ 180°C	[105],[11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.162 W/(m-K) @ 0°C	[48]
	0.1076 @ 12°C	[10]
	0.160 @ 30°C	[48]
Electrical resistivity:	1.282x10 <sup>9</sup> MOhm-m @ 1°C	[10]
	2.7x10 <sup>-6</sup> @ 25°C	[49]
Critical temperature:	280.°C	[108]
	279.°C	[49],[105],[10]
	273.°C	[107]
Critical pressure:	7.9 MPa	[49],[105],[10]
	7.7	[107]
	7.38	[108]
Dynamic viscosity:	0.514 mPa-s @ -13°C	[105]
	0.495 @ -10°C	[105]
	0.4361 @ 0°C	
	0.436 @ 0°C	[105]
	0.433 @ 0°C	[48]
	0.380 @ 5°C	[105]
	0.396 @ 10°C	[48]
	0.3829 @ 15°C	
	0.3683 @ 20°C	
	0.366 @ 20°C	[48]
	0.363 @ 20°C	[10],[105],[108]
	0.341 @ 30°C	[48]
	0.3360 @ 35°C	
	0.330 @ 40°C	[105]
	0.319 @ 40°C	[48]
Kinematic viscosity:	0.407 μm <sup>2</sup> /s @ -13°C	
	0.392 @ -10°C	
	0.3454 @ 0°C	[16]
	0.345 @ 0°C	
	0.343 @ 0°C	
	0.301 @ 5°C	
	0.314 @ 10°C	
	0.3032 @ 15°C	[16]
	0.2916 @ 20°C	[16]
	0.289 @ 20°C	
	0.287 @ 20°C	

# 178 - Carbon disulfide

	0.270	@ 30°C	
	0.2660	@ 35°C	[16]
	0.261	@ 40°C	
	0.256	@ 40°C	
Surface tension:	32. mN/m	@ 20°C	[107]
	32.33	@ 20°C	[105]
	32.25	@ 20°C	[49], [108]
	30.79	@ 30°C	[49]
Contact angle:	unknown		
Thermal expansion coefficient:	0.001218 K <sup>-1</sup>	@ 20°C	[49]
	0.00119	@ 20°C	[48]
Compressibility:	0.795 nPa <sup>-1</sup>	@ 0°C	[105]
	0.854	@ 10°C	[105]
	0.919	@ 20°C	[105]
	0.950	@ 25°C	[49]
	0.996	@ 30°C	[105]
	1.089	@ 40°C	[105]
	1.195	@ 50°C	[105]
Vapor diffusivity:	8.92 μm <sup>2</sup> /s	@ 0°C	[47]
Solution diffusivity:	1.1 nm <sup>2</sup> /s (calc)	in water	[59]
	2.06	50 mol% in toluene	[47]
Electric dipole moment:	0.		[105], [108]
	0.2x10 <sup>-30</sup> C-m		[49], [10]
Ionization potential:	10.4 eV (S)		[105]
Magnetic volume susceptibility:	-8.784x10 <sup>-6</sup> SI units	@ 22°C	[105]
Speed of sound:	1149. m/s	@ 25°C	[105]
Heat of melting:	4.573 kJ/mol		[107]
	4.395		[105]
	4.392		[10]
	4.389		[49]
Heat of vaporization:	27.098 kJ/mol		[107]
	28.4197		[105]
	26.800		[10]
	26.736		[49]
Heat of sublimation:	unknown		
Heat capacity @ 25°C:	0.076 kJ/ (mol-K)	(liq)	
[10], [49], [105]			
	0.0454	(gas)	[105]
	0.0455	(gas)	[10]
Heat of combustion:	-1684.86 kJ/mol	@ 25°C (liq)	[49]
	-1032.5	@ 20°C (liq)	[105]
	-1029.41	@ 25°C (liq)	[107]
Heat of formation:	89.70 kJ/mol	@ 25°C (liq)	[49]
	89.76	(liq)	[10], [105]
	117.36	(gas)	[49]
	117.44	(gas)	[105]
	117.15	(gas)	[10]
Gibbs (free) energy:	65.31 kJ/mol	@ 25°C (liq)	[10]
	66.95	(gas)	[10]

**Analytical chemistry:**  $P_{oct}$  = 1.84 [104],[41]  
 2.16 (calculated) [104],[41],[59]  
 1.71-4.16 [24]  
 $pK_s$  = unknown  
 $pK_a$  = unknown  
 $pK_{BH}$  = unknown  
 Henry's law constant = 0.142 kPa-m<sup>3</sup>/mol (calc) [24]  
 1.32 (calc) [41]  
 0.544 dimensionless [59]  
 Hydrolysis half-life = unknown

**Electrochemical data:** Unknown

**Clay-organic interaction data:** Inorganic

**Solubility:** Slightly soluble in water. Soluble in chloroform. Miscible with ethanol, ether. [105],[56],[10],[108],[49],[32]

0.294 wt% in water @ 20°C [108]  
 0.29 wt% in water @ 20°C [10]  
 0.210 wt% in water @ 20°C [49]  
 0.2 wt% in water @ 20°C [32]  
 0.23 wt% in water @ 22°C [104]  
 0.119 wt% in water @ 25°C [41]

**Form:** Clear, colorless to yellow liquid. Faintly sweetish, pleasing, and aromatic odor when pure to slightly pungent odor, like that of rotten egg or decaying cabbage, in commercial and reagent grades.  
 [51],[107],[56],[104],[22],[108],[32]

**Use:** Manufacture of viscose rayon, cellophane, carbon tetrachloride, rubber chemicals and flotation chemicals, soil disinfectant, electronic vacuum tubes, optical glass, paints, tallow, textiles, explosives, rocket fuel, putty, ammonium salts, carbanilide, xanthogenates, dyes; solvent for phosphorous, sulfur, bromine, iodine, selenium, fats, resins, cold vulcanized rubber, alkali cellulose, waxes, lacquers, camphor; manufacture of grain fumigants, soil conditioners, herbicides, paper, pharmaceuticals; dry-cleaning; oil extraction; electroplating; chemical analysis; widely used as a pesticide intermediate. Occurs naturally as biogenic emissions from soils and in minute amounts in coal tar and crude petroleum.  
 [56],[104],[22],[108],[32]

**Fire and explosion hazard:** Very high.

Flash point: (CC) -30°C [107],[51],[49],[108]

uel: 50% [107],[51],[105],[55]

73% [10]

lel: 1.3% [107],[51],[55]

1.25% [105]

1.2% [10]

Autoign. temp.: 100°C [107],[22]

125°C [51]

Extremely flammable liquid. Dangerous fire and explosion hazard when exposed to flame, heat, sparks, or friction. Can react vigorously with oxidizing materials. Emits highly toxic fumes of SO<sub>x</sub> and CO when heated to decomposition. Flashback along vapor trail may occur. Contact of the

## 180 - Carbon disulfide

vapor or liquid with a hot electric light bulb could cause ignition. Fight fire with CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. Water and foam may be ineffective on fire. Cool exposed containers with water. [51],[107],[22],[32]

**Incompatibility:** Strong oxidizers; chemically active metals such as sodium, potassium, zinc; azides; organic amines; air; halogens; rust. Reacts violently with Al, Cl<sub>2</sub>, azides, CsN<sub>3</sub>, ClO, ethylamine diamine, ethylene imine, F<sub>2</sub>, Pb(N<sub>3</sub>)<sub>2</sub>, LiN<sub>3</sub>, NO, N<sub>2</sub>O<sub>4</sub>, (H<sub>2</sub>S)<sub>4</sub> + permanganates), potassium, KN<sub>3</sub>, RbN<sub>3</sub>, NaN<sub>3</sub>, Zinc. [51],[56]

**Handling:** Keep away from fire, heat, flame, and sources of ignition. Self-contained breathing apparatus required to prevent inhalation. Prevent any reasonable probability of skin or eye contact (polyurethane coated nylon, natural rubber or latex, neoprene synthetic latex, PVA, viton, or butyl synthetic latex overclothing and gloves; splash-proof chemical goggles). Remove contaminated clothing (to avoid flammability hazard) and clean. Facilities for eye wash and quick body drenching should be available. Use in well-ventilated area (fume hood). Keep container tightly closed. Store in iron, aluminum, glass, porcelain, or Teflon containers in cool, dry, well-ventilated, flammable liquid storage area or cabinet. Store in secure poison area. [107],[53],[56],[32]

**Health effects:** Carbon disulfide is poison and irritant. Routes of entry are inhalation of vapor, percutaneous absorption of liquid or vapor, ingestion and skin and eye contact. Points of attack include central nervous system, peripheral nervous system, cardiovascular system, gastrointestinal system, eyes, kidneys, liver, and skin. The chief toxic effect is on the central nervous system. Liquid or concentrated vapors may cause mild irritation of skin, eyes, mucous membrane, and upper respiratory tract. Other symptoms may include headache, garlicky breath, nausea, vomiting, diarrhea, (even after vapor exposure), and occasionally abdominal pain. Massive acute overexposure may cause weak pulse, palpitations, fatigue, weakness in the legs, unsteady gait, vertigo, mania, hallucinations of sight, hearing, taste and smell followed by CNS depression, respiratory paralysis, and death after coma. In acute poisoning, it acts as a narcotic and anesthetic with death following from respiratory failure. In chronic poisoning, it causes central and peripheral damage to the central nervous system, which may become permanent, such as insomnia, nightmares, defective memory, and impotency. Following repeated exposures, subjective psychological and behavioral disorders may be observed. Atherosclerosis and coronary heart disease have been significantly linked to CS<sub>2</sub> exposure. [51],[107],[56],[32]

**Toxicity:** High.TWA: 10 ppm (30 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: 30 ppm (90 mg/m<sup>3</sup>) [51],[56]IDLH: 500 ppm (1550 mg/m<sup>3</sup>) [56],[107]Peak: 100 ppm (310 mg/m<sup>3</sup>) for 30 min [51],[56]Odor threshold: 0.01-1 ppm (0.05-3 mg/m<sup>3</sup>) [104]1 ppm (3 mg/m<sup>3</sup>) -- sense of smell fatigues rapidly [56]0.21 ppm (0.65 mg/m<sup>3</sup>) [107]0.0011-7.7 ppm (0.005-0.32 mg/m<sup>3</sup>) [32]

Carcinogenicity: insufficient data [51]

Mutagenicity: laboratory experiments have shown mutagenic effects [55]  
possible teratogen [55]**Exposure:****External:**Non-lethal: 30 ppm (90 mg/m<sup>3</sup>) -- eye irritation [51]

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: 14 mg/kg body wt -- death of an adult human [51]

186 mg/kg body wt -- death of an adult male [51]

**Inhalation:**Short-term Inhalation Limits: 200 ppm (620 mg/m<sup>3</sup>) for 10 min [107]100 ppm (310 mg/m<sup>3</sup>) for 30 min [107]50 ppm (155 mg/m<sup>3</sup>) for 60 min [107]Non-lethal: <10 ppm (30 mg/m<sup>3</sup>) -- unsatisfactory [104]150 ppm (480 mg/m<sup>3</sup>) -- symptoms of illness [104]500 ppm (1550 mg/m<sup>3</sup>) -- severe toxic effects [104]Lethal: 4000 ppm (12,400 mg/m<sup>3</sup>) for 30 min [51]2000 ppm (6200 mg/m<sup>3</sup>) for 5 min [55]

## 182 - Carbon Tetrachloride

Carbon Tetrachloride

CCl<sub>4</sub>

CAS RN: 56-23-5

Syn: Carbon tetrachloride \* Methane, tetrachloro- \* Asordin \* Benзиноform  
 \* Carbona \* Carbon chloride \* Carbon tet \* ENT 4705 \* ENT 27164 \* Fasciolin  
 \* Flukoids \* Freon 10 \* Katarine \* Methane tetrachloride \* Necatorina \*  
 Necatorine \* Perchloromethane \* Phoenipine \* Pyrene \* R 10 \* RCRA Waste  
 Number U211 \* Spectral \* Tetra \* Tetrachlorocarbon \* Tetrachloromethane \*  
 Tetracol \* Tetrafinol \* Tetraform \* Tetrasol \* UN 1846 (DOT) \* Univerm \*  
 Vermoestricid \*

Molecular formula: CCl<sub>4</sub>

Polychlorinated Aliphatic Halide

### Physical properties:

Relative molecular mass:	153.823	
Specific gravity:	1.597	[51]
	1.595	[48]
	1.59402	[49]
	1.5940	[105], [10], [106]
	1.59	[104], [32]
Boiling point:	1.5867	[10]
	76.8°C	[51], [32], [105]
	76.74°C	[22]
	76.7°C	[10], [104], [48]
	76.638°C	[49]
	76.54°C	[105]
	76.5°C	[107], [106]
Melting point:	-22.6°C	[51]
	-22.8°C	[48]
	-22.82°C	[49]
	22.9°C	[10]
	-22.96°C	[10]
	-22.99°C	[105]
	-23.0°C	[104], [107], [22], [105], [32]
Refractive index:	1.4607	[22]
	1.46018	[49]
	1.4601	[10], [105], [106]
Vapor pressure:	2.51 kPa @ -10°C	(18.81mm) [41]
	4.41 @ 0°C	(33.08mm) [41]
	5.33 @ 4.3°C	(40mm) [105]
	7.5 @ 10°C	(56mm) [104]
	12.0 @ 20°C	(90mm) [104]
	12.13 @ 20°C	(91mm) [32]
	12.17 @ 20°C	(91.3mm) [22]
	13.33 @ 23°C	(100mm) [51], [105]
	15.1 @ 25°C	(113mm) [104]
	15.36 @ 25°C	(115.2mm) [49]
Vapor density:	18.3 @ 30°C	(137mm) [104]
	5.5	[104]
	5.32	[105], [55]
Evaporation rate:	5.3	[107], [22], [32]
	12.8	[32]
	6.0	[49]
	0.33	[3]

## Carbon Tetrachloride - 183

Relative dielectric permittivity:	2.3212	@ -19.8°C	[2]
	2.3170	@ -18.0°C	[2]
	2.3097	@ -14.2°C	[2]
	2.3035	@ -11.0°C	[2]
	2.2997	@ -9.3°C	[2]
	2.2828	@ -5.8°C	[2]
	2.2811	@ 0.0°C	[2]
	2.2758	@ 2.7°C	[2]
	2.2689	@ 6.0°C	[2]
	2.2628	@ 8.7°C	[2]
	2.2586	@ 11.1°C	[2]
	2.2544	@ 13.2°C	[2]
	2.2448	@ 18.0°C	[2]
	2.24	@ 20°C (1 MHz)	[2]
	2.238	@ 20°C	[105], [11], [10]
	2.23790	@ 20°C	[49]
	2.2369	@ 21.8°C	[2]
	2.230	@ 25°C (1 MHz)	[2]
	2.228	@ 25°C (4.5 MHz)	[2]
	2.2288	@ 25°C	[49]
	2.228	@ 25°C	[11]
	2.217	@ 30°C	[2]
	2.205	@ 35°C	[2]
	2.197	@ 40°C	[2]
	2.1887	@ 45°C	[2]
	2.184	@ 50°C	[2]
	2.1688	@ 55°C	[2]
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	0.113	W/(m-K) @ -20°C	[20]
	0.109	@ 0°C	[20], [48]
	0.1055	@ 12°C	[10]
	0.105	@ 20°C	[20]
	0.1034	@ 20°C	[105]
	0.101	@ 40°C	[20]
	0.107	@ 50°C	[48]
	0.09768	@ 50°C	[105]
	0.0972	@ 60°C	[20]
	0.105	@ 100°C	[48]
Electrical resistivity:	2.5x10 <sup>9</sup>	MOhm-m @ 18°C	[10], [49]
Critical temperature:	283.4°C		[49]
	283.15°C		[10]
	283.1°C		[105]
	283.°C		[107]
Critical pressure:	4.6	MPa	[107]
	4.56		[105], [10]
	4.516		[49]

# 184 - Carbon Tetrachloride

Dynamic viscosity:	1.680 mPa-s	@ -10°C	[48]
	1.329	@ 0°C	[105], [48]
	1.130	@ 10°C	[48]
	1.038	@ 15°C	[105]
	0.9715	@ 20°C	
	0.969	@ 20°C	[105], [48]
	0.965	@ 20°C	[10]
	0.9004	@ 25°C	[49]
	0.843	@ 30°C	[105], [48]
	0.75546	@ 40°C	
	0.739	@ 40°C	[105], [48]
	0.651	@ 50°C	[105], [48]
	0.585	@ 60°C	[105], [48]
	0.524	@ 70°C	[105], [48]
	0.468	@ 80°C	[105], [48]
	0.426	@ 90°C	[105], [48]
	0.384	@ 100°C	[105], [48]

Kinematic viscosity:	1.053 $\mu\text{m}^2/\text{s}$	@ -10°C	
	0.834	@ 0°C	
	0.708	@ 10°C	
	0.651	@ 15°C	
	0.6091	@ 20°C	[15]
	0.608	@ 20°C	
	0.605	@ 20°C	
	0.5649	@ 25°C	
	0.529	@ 30°C	
	0.47364	@ 40°C	[15]
	0.464	@ 40°C	
	0.408	@ 50°C	
	0.367	@ 60°C	
	0.329	@ 70°C	
	0.294	@ 80°C	
	0.267	@ 90°C	
	0.241	@ 100°C	

Surface tension: ([10] values are calculated)	29.49 mN/m	@ 0°C	[10]
	29.43	@ 10°C	[10]
	27.	@ 20°C	[107]
	26.95	@ 20°C vapor	[105]
	26.92	@ 20°C	[49]
	26.13	@ 25°C	[49]
	25.82	@ 30°C	[10]
	24.59	@ 40°C	[10]
	23.37	@ 50°C	[10]
	22.15	@ 60°C	[10]
	17.26	@ 100°C	[105]
	6.53	@ 200°C	[105]

Contact angle: [18]

	sessile	advancing	receding
quartz	9	12	8
calcite	13	18	9
biotite	11	14	8
Ca-mont.	6	9	6



Thermal expansion coefficient:	0.001229 K <sup>-1</sup> @ 25°C	[49]
	0.00122 @ 20°C	[48]
Compressibility:	0.885 nPa <sup>-1</sup> @ 0°C	[105]
	0.945 @ 10°C	[105]
	1.04 @ 20°C	[105]
	1.0799 @ 25°C	[49]
	1.128 @ 30°C	[105]
	1.220 @ 40°C	[105]
	1.320 @ 50°C	[105]
	1.426 @ 60°C	[105]
	1.543 @ 70°C	[105]
Vapor diffusivity:	29.3 μm <sup>2</sup> /s @ 0°C in H <sub>2</sub>	[47]
	6.36 @ 0°C in O <sub>2</sub>	[47]
Solution diffusivity:	2.04 nm <sup>2</sup> /s in benzene	[47]
	1.49 in cyclohexane	[47]
	0.776 in decalin	[47]
	1.02 in dioxane	[47]
	1.5 in ethanol	[47]
	3.17 in n-heptane	[47]
	0.961 in kerosene	[47]
	2.30 in methanol	[47]
	2.57 in i-octane	[47]
	0.735 in tetralin	[47]
Electric dipole moment:	0	[49], [105], [10]
Ionization potential:	11.47 eV (PI)	[105]
Magnetic volume susceptibility:	-0.691x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	926. m/s @ 25°C	[105]
	852. @ 50°C	[20]
Heat of melting:	3.276 kJ/mol	[105]
	2.516	[10]
	2.43	[49]
Heat of vaporization:	34.631 kJ/mol	[105]
	31.940	[105]
	30.135	[107]
	29.98	[10]
	29.96 @ bp	[49]
	32.41 @ 25°C	[49]
Heat of sublimation:	32.62 kJ/mol	[10]
Heat capacity @ 25°C:	0.1318 kJ/(mol-K) (liq)	[105]
	0.13136 (liq)	[49]
	0.0835 (gas)	[10]
	0.0833 (gas)	[105]
Heat of combustion:	-258.24 kJ/mol @ 25°C (liq)	[20]
	-290.98 (gas)	[20]
	-156.2 @ 20°C (liq)	[105]
Heat of formation:	-135.44 kJ/mol @ 25°C (liq)	[49]
	-135.53 (liq)	[105]
	-132.9 (liq)	[10]
	-103.00 (gas)	[105]
	-95.87 (gas)	[10]
	-95.81 (gas)	[49]

## 186 - Carbon Tetrachloride

Gibbs (free) energy:	-62.68 kJ/mol @ 25°C (liq)	[10]
	-65.31 (liq)	[105]
	-53.59 (gas)	[10]
	-60.67 (gas)	[105]
Analytical chemistry: $pP_{oct}$ =	2.96	[31]
	2.83	[21], [24]
	2.73	[4]
	2.64 @ 20°C	[104], [8], [27]
	2.62	[21]
	2.35	[41]
	$pK_s$ = unknown	
	$pK_a$ = NA	[31]
	$pK_{BH}$ = unknown	
	Henry's law constant = 3.08 kPa-m <sup>3</sup> /mol @ 24.8°C	[24]
Hydrolysis half-life =	3.06	[41]
	2.33	[41]
	2.43 @ 20°C	[41]
	10.3 @ 37°C	[41]
	2.2x10 <sup>11</sup> sec (1 ppm)	[13]
	2.2x10 <sup>8</sup> to 2.2x10 <sup>11</sup> sec	[8]

**Electrochemical data:** Meites and Zuman (1977), Meites et al. (1977a), Meites et al. (1977b).

**Clay-organic interaction data:** Carbon tetrachloride increases the hydraulic conductivity of clay soil (Evans et al., 1985). Sorption on soil and clay (Rogers and McFarlane, 1981).

**Solubility:** Practically insoluble in water. Miscible with ethanol, acetone, ether, benzene, chloroform, solvent naphtha, petroleum ether, most fixed and volatile oils. [105],[22]

0.097 wt% in water @ 0°C	[10]
0.08 vol% in water @ 20°C	[104]
0.08 wt% in water @ 20°C	[32]
0.077 wt% in water @ 25°C	[49]
0.116 wt% in water @ 25°C	[104]

**Form:** Colorless liquid. Sweetish, aromatic, moderately strong, ether-like or chloroform-like odor. [51],[107],[56],[22],[32]

**Use:** Manufacture of fluorocarbons for aerosols, refrigerants and fire extinguishments; as an agricultural grain fumigant and pesticide; in polymer technology as reaction medium, catalyst and chain transfer agent, and solvent for resins; organic synthesis for chlorination of organic compounds in soap perfumery and insecticide industries; industrial solvent for rubber cements, cable and semiconductor manufacture, and separation of xylene isomers as components to reduce flammability; laboratory solvent; in metal recovery and catalyst regeneration; for cleaning clothing; rendering benzin nonflammable; azeotropic drying agent for wet spark plugs in automobiles; solvent for oils, fats, lacquers, varnishes, rubber waxes, resins; extracting oil from flowers and seeds; exterminating destructive insects. Banned from household use by the FDA. Banned by the EPA on 12/31/85 as a fumigant. [56],[104],[22],[5],[32]

**Fire and explosion hazard:** Very low.

Flash point: NA

UEL: NA

LEL: NA

Autoign. temp.: NA

Nonflammable liquid. If heated, may decompose forming toxic gases and vapors such as phosgene, chlorine gas, hydrogen chloride, carbon monoxide, and hydrochloric acid. Stop discharge if possible. Do not use to put out fires. [51],[107],[32]

**Incompatibility:** Chemically active metals such as sodium, potassium and magnesium; aluminum trichloride, calcium disilicide, chlorine trifluoride, decaborane (14), dibenzoyl peroxide, N-N-dimethylformamide, 1,2,3,4,5,6-hexachlorocyclohexane; dinitrogen tetroxide, fluorine, metals, potassium-tert-butoxide. Severe reaction with allyl alcohol, Al,  $\text{Al}(\text{C}_2\text{H}_5)_3$ , Ba, (benzoyl peroxide +  $\text{C}_2\text{H}_4$ ), Be,  $\text{BrF}_3$ ,  $\text{Ca}(\text{OCl})_2$ , diborane,  $\text{C}_2\text{H}_4$ , dimethyl formamide, disilane,  $\text{F}_2$ , Li, Mg, liquid  $\text{O}_2$ , Pu, K, ( $\text{AgClO}_4 + \text{HCl}$ ), Na, NaK, tetrasilane, trisilane, U, Zr, burning wax. [51],[56]

**Handling:** Keep away from heat, flame and sources of ignition. Do not breath vapors. Organic vapor canister respirator with full mask or self-contained breathing apparatus required. Prevent any reasonable probability of eye contact (chemical safety goggles and face shield). Prevent repeated or prolonged skin contact (nitrile or PVA synthetic or viton latex gloves and protective suit). Use with adequate ventilation (fume hood). Remove contaminated clothing promptly if wet or contaminated and clean. Keep container tightly closed. Store in cool, dry, secure poison area. [107],[53],[56],[32]

**Health effects:** Carbon tetrachloride is a poison, experimental mutagen, and suspected human carcinogen. Routes of entry are inhalation of vapor, percutaneous absorption, ingestion, and skin and eye contact. Points of attack include central nervous system, eyes, lungs, liver, kidneys, and skin. Exposure may cause headache, drowsiness, nausea, vomiting, epigastric distress, loss of appetite, fatigue, dizziness, incoordination and unconsciousness. Inhalation of the vapors may cause severe irritation of the respiratory system and mucous membranes. Eye contact with the liquid causes burning and intense irritation. Delayed effects of short-term exposure include damage to the heart, liver and kidneys. Chronic effects of overexposure may include kidney and/or liver damage and CNS depression. Symptoms of liver damage include yellow jaundice and dark urine. Prolonged or repeated contact with the skin may cause dermatitis. Alcoholism and previous liver and kidney damage seem to render an individual more susceptible. The narcotic action resembles that of chloroform though not as strong. This substance has been listed as a carcinogen by the EPA. It is a common air and water contaminant. [51],[107],[56],[32],[55],[64]

## 188 - Carbon Tetrachloride

### Toxicity: Very high.

TWA: 5 ppm (30 mg/m<sup>3</sup>) (skin) -- suspected human carcinogen [1]

STEL: no value set [1]

CL: 25 ppm (155 mg/m<sup>3</sup>) [51]

IDLH: 300 ppm (1890 mg/m<sup>3</sup>) [107],[56]

Peak: 200 ppm (1260 mg/m<sup>3</sup>) for 5 min in a 4 hr period if no other measurable exposure occurs [51]

Odor threshold: 16-480 ppm (100-3000 mg/m<sup>3</sup>) [104]

50 ppm (310 mg/m<sup>3</sup>) [32]

Carcinogenicity: human suspected, animal positive. [1],[51],[56]

Mutagenicity: experimental teratogen, equivalent tumorigenic agent, neoplastic effects, Negative *Salmonella* tests. [51],[104] nonmutagenic [30]

### Exposure:

#### External:

Non-lethal: unknown

Lethal: 1000-2000 ppm (6300-12600 mg/m<sup>3</sup>) for 1/2 to 1 hr -- death from acute renal damage [51]

#### Oral:

Non-lethal: 1800 mg/kg body wt -- Pulmonary and systemic effects [51]

1700 mg/kg body wt -- CNS effects [51]

Lethal: 43 mg/kg body wt -- death of an adult human [51]

93 mg/kg body wt -- death of an adult male [51]

#### Inhalation:

Short-term Inhalation Limits: 25 ppm (155 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: 10 ppm (63 mg/m<sup>3</sup>) -- no adverse symptoms [51]

20 ppm (125 mg/m<sup>3</sup>) -- toxic CNS effects [51]

25-30 ppm (155-190 mg/m<sup>3</sup>) -- adverse effects [51]

>50 ppm (315 mg/m<sup>3</sup>) -- unsatisfactory [104]

317 ppm for 30 min--Gastrointestinal tract effects [51]

500 ppm (3200 mg/m<sup>3</sup>) -- symptoms of illness begin [104]

1000-1500 ppm (6300-9450 mg/m<sup>3</sup>) for several hours --

sufficient to cause symptoms [104]

2000 ppm (12.6 g/m<sup>3</sup>)/60 min -- severe toxic effects [104]

Lethal: 1000 ppm (6300 mg/m<sup>3</sup>) -- death of an adult human [51]

5 ppm (30 mg/m<sup>3</sup>) for 5m [55]

Chlordane

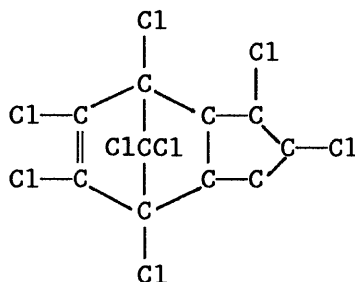
 $C_{10}H_6Cl_8$ 

CAS RN: 57-74-9

Syn: Chlordane \* 4,7-Methano-1H-indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro- \* Belt \* CD-68 \*  $\gamma$ -Chlordan \* gamma-Chlordan \* Chlorindan \* chlorodane \* Corodane \* Cortilan-neu \* Dowklor \* ENT 9932 \* ENT 25,552-x \* HCS-3260 \* M-140 \* 4,7-Methanoindan, 1,2,4,5,6,7,8,8-octachloro-3a,4,7,7a-tetrahydro- \* NCI-C00099 \* Niran \* Octachlorodihydrodicyclopentadiene \* 1,2,4,5,6,7,8,8-Octachloro-2,3,4a,4,7,7a-hexahydro-4,7-methanoindene \* 1,2,4,5,6,7,8,8-Octachloro-2,3,4a,4,7,7a-hexahydro-4,7-methano-1H-indene \* 1,2,4,5,6,7,8,8-Octachloro-3a,4,7,7a-hexahydro-4,7-methylene indane \* Octachloro-4,7-methanohydroindane \* Octachloro-4,7-methanotetrahydroindane \* 1,2,4,5,6,7,8,8-Octachloro-4,7-methano-3a,4,7,7a-tetrahydroindane \* 1,2,4,5,6,7,8,8-Octachloro-3a,4,7,7a-tetrahydro-4,7-methanoindane \* 1,2,4,5,6,7,10,10-Octachloro-4,7,8,9-tetrahydro-4,7-methyleneindane \* Octachlor \* Octa-klor \* Oktaterr \* Ortho-Klor \* Synklor \* Tat Chlor 4 \* Toxichlor \* Velsicol 1068 \* 1068 \*

**Structural formula:**

Chlorinated Polycyclic Hydrocarbon

**Physical properties:**

Relative molecular mass:	409.782	
Specific gravity:	1.57-1.63 (15.5/15.5)	[51]
	1.6 @ 25°C	[107]
	1.59-1.63 @ 25°C	[108]
	1.57-1.67 (60/60)	[22]
Boiling point:	175.°C @ 0.267 kPa (2mm)	[22], [51], [32]
	decomposes	[107], [32]
Melting point:	103.-108°C	[31]
Refractive index:	1.56-1.57 @ 25°C	[22], [108]
Vapor pressure:	1.33x10 <sup>-6</sup> kPa @ 20°C (1x10 <sup>-5</sup> mm)	[32]
	1.33x10 <sup>-6</sup> @ 25°C (1x10 <sup>-5</sup> mm)	[65]
Vapor density:	14.15 @ 25°C	[41]
	14. @ bp	[32]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	1.104 mPa-s @ 25°C	
Kinematic viscosity:	0.69 $\mu m^2/s$ @ 25°C	[108]
Surface tension:	25. mN/m @ 20°C	[107]

## 190 - Chlordane

Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	unknown	
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	unknown	
Heat of combustion:	3811. kJ/mol (est) (liq)	[107]
Heat of formation:	unknown	
Gibbs (free) energy:	unknown	

Analytical chemistry: $pP_{oct}$ =	6.00	[41]
	5.48	[31]
	3.32	[65]
	2.78	[8]
$pK_s$ =	NA	
$pK_a$ =	NA	[31]
$pK_{BH}$ =	NA	
Henry's law constant =	0.00486 kPa-m <sup>3</sup> /mol	[41]
Hydrolysis half-life =	>1.3x10 <sup>8</sup> sec	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

**Solubility:** Practically insoluble in water. Soluble in many organic solvents. Miscible with deodorized kerosene, aliphatic and aromatic hydrocarbon solvents. Decomposes in weak alkalis. [22],[108]

5.6x10 <sup>-6</sup> vol% <i>cis:trans</i> (75:25)	
in water	[104]
9.x10 <sup>-7</sup> wt% technical in water	[104]

**Form:** Colorless to amber or brown, viscous liquid. Odorless to penetrating and aromatic; slightly pungent like chlorine. Shipped as a variety of dusts and powders, and as solutions in kerosene containing 2-80% chlordane. [51],[107],[104],[56],[32]

Technical chlordane consists of 60-70% isomers of chlordane and 25-40% of related compounds including 2 isomers of heptachlor and one each of enneachloro- and decachlorodicyclopentadiene. Two isomers of octachlorodicyclopentadiene have been isolated from chlordane of which  $\alpha$ -chlordane is the *endo-cis* and  $\beta$ -chlordane is the *endo-trans* isomer. The commercial product known as  $\gamma$ -chlordane is substantially the  $\alpha$ -isomer. Technical chlordane is a mixture of 26 organochlorine compounds. [104],[108]

Approximate composition of technical chlordane [104]:

<u>fraction</u>	<u>percent present</u>
<i>cis</i> (a)chlordane ( $C_{10}H_6Cl_8$ )	$19 \pm 3$
<i>trans</i> (c)chlordane ( $C_{10}H_6Cl_8$ )	$24 \pm 2$
chlordene (4 isomers) ( $C_{10}H_6Cl_6$ )	$21.5 \pm 5$
heptachlor ( $C_{10}H_5Cl_7$ )	$10 \pm 3$
nonachlor ( $C_{10}H_5Cl_9$ )	$7 \pm 3$
( $C_{10}H_7-8Cl_{6-7}$ )	$8.5 \pm 2$
hexachlorocyclopentadiene ( $C_5Cl_6$ )	>1
octachlorocyclopentadiene ( $C_5Cl_8$ )	$1 \pm 1$
Diels-Adler adduct of cyclopentadiene and pentachlorocyclopentadiene ( $C_{10}H_6Cl_5$ )	$2 \pm 1$
others	$6 \pm 5$

**Use:** Non-systemic, broad spectrum insecticide (slightly more toxic than DDT) for termite control, in homes and gardens, in crop production for soil insects (fire and harvester ants). Use has been suspended by the EPA, except for commercial use in termite control, as of 1980. [51],[108],[5],[32]

**Fire and explosion hazard:** Low.

Flash point: (CC) 55.6°C in kerosene solution [107]

(OC) 107°C in kerosene solution [107]

uel: 5% in kerosene solution [107]

lel: 0.7% in kerosene solution [107]

Autoign. temp.: 210°C in kerosene solution [107]

Combustible liquid. Solid is not flammable. May emit irritating and toxic fumes of hydrogen chloride, phosgene, carbon monoxide, and chlorine when heated to decomposition (>200°C). Fight fire with dry chemicals, foam, CO<sub>2</sub>. Stop discharge if possible. Water may be ineffective on fire. Cool exposed containers with water. [51],[107],[32]

**Incompatibility:** No reaction with common materials. Contact with strong oxidizers may cause fires and explosions. Will attack some plastics, rubber, and coatings. [107],[56],[32]

**Handling:** Appropriate respirator or self-contained breathing apparatus required to prevent inhalation. Prevent any possibility of skin or eye contact (vinyl plastic, nitrile or natural rubber or latex overclothing and gloves). Remove contaminated clothing and shoes. Facilities for eye wash and quick body drenching should be available. Store in aluminum, aluminum-clad or phenolic enamel-lined metal containers in secure poison area. [32],[56],[107]

**Health effects:** Chlordane is a poison and experimental human carcinogen. Routes of entry are inhalation, skin absorption, ingestion and skin and eye contact. Points of attack include the central nervous system, eyes, lungs, liver, kidneys, and skin. It is a CNS stimulant whose exact mode of action is unknown. It is moderately irritating to the eyes and skin. Symptoms of overexposure include blurred vision, confusion, ataxia, delirium, coughing, anuria, excitability, convulsions, nausea, vomiting, diarrhea, and some local irritation of the gastrointestinal tract. [51],[107],[108],[32],[65]

## 192 - Chlordane

### Toxicity: Very high.

TWA: 0.03 ppm (0.5 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 30 ppm (500 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: unknown

Carcinogenicity: human experimental; animal positive [51],[32]  
human leukemia and blood dyscrasia [17]

Mutagenicity: human potential [51]  
positive [37]

### Exposure:

#### External:

Non-lethal: unknown

Lethal: 30 g of technical chlordane on skin -- death of an adult human  
in 40 min [32],[51]

#### Oral:

Non-lethal: unknown

Lethal: 2-4 g [51]

6-60 g (0.2-2 oz) [51]

40 mg/kg body wt -- death of an adult human [51]

118 mg/kg body wt -- death of an adult male [51]

104 mg/kg body wt (6 g) -- by suicidal adult human [32]

#### Inhalation:

Short-term Inhalation Limits: 0.12 ppm (2 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: unknown

Lethal: unknown



Chlorobenzene

 $C_6H_5Cl$ 

CAS RN: 108-90-7

Syn: Chlorobenzene \* Benzene, chloro- \* Benzene chloride \* Chlorobenzene \* Chlorbenzol \* Chlorobenzol \* MCB \* Monochlorbenzene \* Monochlorbenzol \* Monochlorobenzene \* NCI-C54886 \* Phenyl chloride \* RCRA Waste Number U037 \* Tetrosin SP \* UN 1134 (DOT) \*

Molecular formula:  $C_6H_5Cl$ 

Chlorinated Aromatic Hydrocarbon

## Physical properties:

Relative molecular mass:	112.559	
Specific gravity:	1.11	[107]
	1.1	[32]
	1.1066	[104]
	1.1063	[49], [10]
	1.106	[48]
	1.1058	[105], [106]
Boiling point:	132.°C	[104], [105], [107], [48], [32]
	131.7°C	[10], [51]
	131.687°C	[49]
	131.6°C	[22]
	131.°-132°C	[56]
Melting point:	-44.°C	[32]
	-45.°C	[104], [51], [48], [22]
	-45.3°C	[10]
	-45.58°C	[49]
	-45.6°C	[105], [107], [106]
Refractive index:	1.52481	[49]
	1.5248	[10]
	1.5241	[105], [106]
Vapor pressure:	0.1333 kPa @ -13°C	(1mm) [105]
	0.4 @ 0°C	(3mm) [41]
	1.17 @ 20°	(8.8mm) [104], [32]
	1.333 @ 22.2°C	(10mm) [105], [51]
	1.567 @ 25°C	(11.75mm) [49]
	1.57 @ 25°C	(11.8mm) [104]
	1.58 @ 25°C	11.9mm) [23]
	2.00 @ 30°C	(15mm) [104]
	5.333 @ 49.7°C	(40mm) [105]
Vapor density:	3.9	[32]
	3.88	[104], [51]
Evaporation rate:	1.07	[3]
	1.	[32]
Relative dielectric permittivity:	6.30 @ -20°C	[105], [11]
	5.95 @ -10°C	[2]
	5.83 @ 0°C	[2]
	5.72 @ 10°C	[2]
	5.71 @ 20°C	[105], [11]
	5.70 @ 20°C	(1.8 MHz) [2]
	6.69 @ 20°C	(1 MHz) [2]
	5.60 @ 20°C	(500 MHz) [2]
	5.57 @ 20°C	(2.4 GHz) [2]
	5.621 @ 25°C	[49], [105], [14]
	5.62 @ 25°C	[10], [11]

# 194 - Chlorobenzene

	5.61 @ 25°C (28 MHz)	[2]	
	5.552 @ 30°C	[49]	
Loss tangent:	unknown		
Relaxation time:	10.3x10 <sup>-12</sup> sec	[19]	
Thermal conductivity:	0.151 W/(m-K) @ 0°C	[48]	
	0.127 @ 12°C	[48]	
	0.126 @ 12°C	[10]	
	0.138 @ 75°C	[48]	
	0.1447 @ 30°-100°C	[105]	
Electrical resistivity:	143. MOhm-m @ 25°C	[49]	
	>10. @ 0°C	[11]	
Critical temperature:	359.2°C	[49], [105], [10]	
	359.°C	[107]	
Critical pressure:	4.519 MPa	[105], [10]	
	4.52	[49], [107]	
Dynamic viscosity:	1.06 mPa-s @ 0°C	[48]	
	0.907 @ 10°C	[48]	
	0.900 @ 15°C	[105]	
	0.799 @ 20°C	[10], [105], [48]	
	0.7184 @ 30°C	[49]	
	0.631 @ 40°C	[105]	
	0.567 @ 50°C	[48]	
	0.515 @ 60°C	[48]	
	0.471 @ 70°C	[48]	
	0.431 @ 80°C	[105], [48]	
Kinematic viscosity:	0.958 μm <sup>2</sup> /s @ 0°C		
	0.820 @ 10°C		
	0.814 @ 15°C		
	0.723 @ 20°C		
	0.6497 @ 30°C		
	0.571 @ 40°C		
	0.513 @ 50°C		
	0.466 @ 60°C		
	0.426 @ 70°C		
	0.390 @ 80°C		
Surface tension:	33.56 mN/m @ 20°C vapor	[105]	
	33.19 @ 20°C	[14]	
	32.96 @ 20°C	[49]	
	33.0 @ 25°C	[107]	
	31.98 @ 30°C	[49], [14]	
	30.77 @ 40°C	[14]	
Contact angle: [18]			
	sessile	advancing	receding
quartz	14	12	6
calcite	14	15	8
biotite	13	16	6
Ca-mont.	5	10	0
Thermal expansion coefficient:	0.000990 K <sup>-1</sup>	[49]	
	0.00098	[48]	

Compressibility:	0.738 nPa <sup>-1</sup> @ 20°C	[105]
	0.731 @ 20°C	[49]
	0.771 @ 25°C	[49]
	0.784 @ 30°C	[105]
	0.832 @ 40°C	[105]
Vapor diffusivity:	7.5 μm <sup>2</sup> /s @ 30°C	[47], [59]
Solution diffusivity:	0.79 nm <sup>2</sup> /s in water (calc)	[59]
	2.66 in benzene	[47]
Electric dipole moment:	5.637x10 <sup>-30</sup> C-m	[105], [10]
	5.404x10 <sup>-30</sup>	[49]
Ionization potential:	9.07 eV (PI)	[105]
Magnetic volume susceptibility:	-8.65x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	1311. m/s @ 20°C	[20]
	1282. @ 30°C	[20]
	1254. @ 40°C	[20]
	1226. @ 50°C	[20]
	1197. @ 60°C	[20]
Heat of melting:	9.614 kJ/mol	[107]
	9.607	[105]
	9.556	[49]
	9.546	[10]
Heat of vaporization:	42.278 kJ/mol	[105]
	40.97 @ 25°C	[49]
	36.55 @ bp	[49]
	37.693	[105]
	36.55	[10]
	35.35	[107]
Heat of sublimation:	41.07 kJ/mol	[10]
Heat capacity @ 25°C:	0.150 kJ/(mol-K) (liq)	[10]
	0.14883 (liq)	[49]
	0.146 (liq)	[105]
	0.0987 (gas)	[105]
Heat of combustion:	-3088. kJ/mol @ 25°C (liq)	[20]
	-3108.88 (liq)	[49]
	-3130. (gas)	[20]
Heat of formation:	10.80 kJ/mol @ 25°C (liq)	[10]
	10.67 (liq)	[49]
	52.3 (gas)	[20]
Gibbs (free) energy:	89.26 kJ/mol @ 25°C (liq)	[10]
Analytical chemistry: pP <sub>oct</sub> =	2.98	[12], [41]
	2.84 @ 20°C	[104], [23], [8], [21], [31]
	2.71	[41]
	2.46	[21]
	2.18	[21]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	0.375 kPa-m <sup>3</sup> /mol	[41]
	0.451 @ 25°C	[41]
	0.629 @ 37°C	[41]
	0.154 dimensionless	[59]
Hydrolysis half-life =	NA	[8]

## 196 - Chlorobenzene

**Electrochemical data:** Neikam et al. (1964), Sease et al. (1968), Wawzonek and Wagenknecht (1963), Meites and Zuman (1977), Meites et al. (1983)

**Clay-organic interaction data:** Chiou et al. (1983), Greene-Kelly (1955), Serratosa (1968).

**Solubility:** Practically insoluble in water. Very soluble in carbon tetrachloride, carbon disulfide, chloroform. Miscible with benzene, ethanol, ether, acetone, n-heptane, most organic solvents. [105],[22],[14],[10],[32],[104],[49]

0.049	wt% in water @ 20°C	[10]
0.05	wt% in water	[14]
0.05	wt% in water @ 20°C	[104],[32]
0.0488	wt% in water @ 30°C	[104],[49]
0.04717	wt% in water @ 25°C	[23]

**Form:** Clear, colorless liquid. Faint, aromatic, amine-like or almond-like odor. Technical grades are 99.5% pure. [51],[107],[104]

**Use:** Manufacture of phenol, aniline, DDT, picric acid, chloronitrobenzene, betachloroanthraquinone, rubber adhesives, and adhesives; as an intermediate in the manufacture of *ortho*- and *para*-nitrobenzenes for use in dye manufacture; as fiber swelling agent and dye carrier in textile processing; tar and grease remover; solvent in surface coatings and surface coating removers; extractant in manufacture of diisocyanates, rubber, perfumes, and pharmaceuticals. [104],[56],[22],[32]

**Fire and explosion hazard:** High.

Flash point: (CC) 29.4°C [51]  
(CC) 29°C [107],[49]  
(CC) 28.9°C [32]  
(OC) 36°C [107]  
uel: 7.1% @ 150°C [51],[107]  
9.6% [22]  
lel: 1.3% [51],[107]  
1.8% [22]  
Autoign. temp.: 637.8°C [51]  
638°C [32]  
640°C [107]

Flammable liquid. Dangerous fire hazard when exposed to heat, sparks or flame. Flashback along vapor trail may occur. Vapor may explode if ignited in an enclosed area. Moderate explosion hazard when exposed to heat or flame. May emit highly toxic fumes of hydrogen chloride, phosgene, and carbon monoxide. Can react vigorously with oxidizing materials. Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder (water spray to blanket fire). Water may be ineffective. [51],[107],[32],[55]

**Incompatibility:** Strong oxidizers; AgClO<sub>4</sub>; dimethyl sulfoxide; finely divided Na. [51],[56],[32]

**Handling:** Keep away from heat, sparks and flame. Avoid breathing mist or vapor (appropriate respirator or self-contained breathing apparatus). Avoid repeated or prolonged eye or skin contact (neoprene or PVA synthetic latex gloves; lab coat; safety goggles). Remove contaminated clothing and shoes. Use in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Bond and ground containers when transferring liquid. Store in cool, dry, well-ventilated flammable liquid storage area. [107],[56],[32],[55]

**Health effects:** Chlorobenzene is a fairly strong narcotic and possesses only slight irritant qualities. Routes of entry are inhalation, ingestion, skin and eye contact. Points of attack include respiratory system, eyes, skin, central nervous system, and liver. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Short term exposure may cause drowsiness, incoordination, and unconsciousness. Exposures to high levels might also cause liver damage. Prolonged or repeated skin contact may cause skin irritation, burns, or dermatitis due to defatting action. Somnolence, loss of consciousness, twitching of the extremities, cyanosis, deep, rapid respirations and a small, irregular pulse are the chief symptoms occurring in acute exposures. Urine may be burgundy red, the red blood cells show degenerative and regenerative changes. Chronic overexposure can cause liver and/or kidney damage. [51],[107],[56],[32],[55],[66]

**Toxicity:** Moderate.

TWA: 75 ppm (350 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: 2400 ppm (11000 mg/m<sup>3</sup>) [56],[107]

Peak: unknown

Odor threshold: 0.21 ppm (1 mg/m<sup>3</sup>) [107]

0.212-1.52 ppm (1.0-7 mg/m<sup>3</sup>) -- recognition [104]

60 ppm (275 mg/m<sup>3</sup>) [32]

Carcinogenicity: indefinite [26]

Mutagenicity: indefinite [66]

positive [37]

**Exposure:**

External:

Non-lethal: 200 ppm for 60 min -- eye and nasal irritation [32]

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: >75 ppm (350 mg/m<sup>3</sup>) -- unsatisfactory [104]

400 ppm for 60 min -- severe toxic effects [104]

Lethal: unknown

198 - 6-Chloro-*m*-cresol6-Chloro-*m*-cresolC<sub>7</sub>H<sub>7</sub>ClO

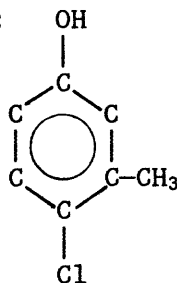
CAS RN: 59-50-7

Syn: 6-Chloro-*m*-cresol \* Phenol, 4-chloro-3-methyl- \* Aptal \* Baktol \* Baktolan \* Canaseptic \* *p*-Chloro-*m*-cresol \* *para*-Chloro-*meta*-cresol \* *p*-Chlor-*m*-cresol \* Chlorocresol \* *p*-Chlorocresol \* 4-Chloro-*m*-cresol \* 4-Chloro-1-hydroxy-3-methylbenzene \* 6-Chloro-3-hydroxytoluene \* 4-Chloro-3-hydroxytoluene \* 2-Chloro-hydroxytoluene \* 2-Chloro-5-methylphenol \* 4-Chloro-3-methylphenol \* *m*-Cresol, 4-chloro- \* 3-Methyl-4-chlorophenol \* Ottafact \* Parmetol \* Parol \* PCMC \* Peritonan \* Preventol CMK \* Raschit \* Raschit K \* Rasen-Anicon \* RCRA Waste Number U039 \*

Molecular formula: CH<sub>3</sub>-C<sub>6</sub>H<sub>3</sub>(OH)Cl

Chlorinated Phenol

Structural formula:

**Physical properties:**

Relative molecular mass:	142.585	
Specific gravity:	1.215 @ 15°C	[105]
Boiling point:	235.°C	[10], [104], [51], [22], [108]
	196.°C	[105]
Melting point:	68.°C	[10]
	66.°C	[104], [51], [108]
	64.°-66.°C	[22]
	55.5°C	[108]
	55.°-56°C	[56]
	45.°-46°C	[105]
Refractive index:	unknown	
Vapor pressure:	0.00667 kPa @ 20°C (0.05mm)	[41], [31]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	

Magnetic volume susceptibility	unknown
Speed of sound:	unknown
Heat of melting:	unknown
Heat of vaporization:	unknown
Heat of sublimation:	unknown
Heat capacity @ 25°C:	unknown
Heat of combustion:	unknown
Heat of formation:	unknown
Gibbs (free) energy:	unknown

Analytical chemistry:	pP <sub>oct</sub> =	3.10	[104], [21]
		2.95	[8], [31], [41]
	pK <sub>s</sub> =	NA	
	pK <sub>a</sub> =	NA	[31]
		9.549	[41]
	pK <sub>BH</sub> =	NA	
	Henry's law constant =	1.78x10 <sup>-6</sup> am-m <sup>3</sup> /mol (calc)	[41]
	Hydrolysis half-life =	NA	[8]

**Electrochemical data:** Unknown

Clay-organic interaction data: Unknown

**Solubility:** Practically insoluble in water (more soluble in hot water). Soluble in benzene, ethanol, chloroform, ether, acetone, ether, aqueous alkaline solutions, fats oils, organic solvents, fixed oils, terpenes. [51],[22],[10],[108]

0.004 vol% in water @ 25°C [22]  
0.0038 wt% in water @ 20°C [108]

**Form:** Colorless, white or slightly pink crystals (solid). Slowly turns light brown on exposure to air. Slight phenolic odor. Odorless when pure. [51], [104], [56], [22], [108], [41]

**Use:** External germicide; preservative for glues, gums, inks, textile and leather goods; preservative in cosmetics; topical antiseptic (veterinarian); disinfectant. [104],[56],[22],[41]

**Fire and explosion hazard:** Unknown

Flash point: unknown

uel: unknown

le1: unknown

Autoign. temp.: unknown

May emit toxic fumes of phosgene, carbon monoxide, carbon dioxide, or hydrogen chloride gas when heated to decomposition. [51], [55]

**Incompatibility:** Bases; acid chlorides; acid anhydrides; oxidizing agents; corrodes steel; brass; copper; copper alloys. [55]

**Handling:** Wear appropriate respirator or self-contained breathing apparatus to avoid inhalation of dust or fumes. Avoid prolonged skin or eye contact (rubber boots and heavy rubber gloves, safety goggles). Safety shower and eye bath should be provide. Keep container tightly closed. Store in a cool, dry, secure poison area. [55]

## 200 - 6-Chloro-*m*-cresol

**Health effects:** Very little data are available concerning the toxicity and health effects of PCMC. It may be an allergen. Routes of entry are inhalation, ingestion, and skin absorption. Points of attack include upper respiratory system, eyes. One source has rated it as very toxic with a probable lethal dose to humans or 50 to 500 mg/kg. It is reported as nonirritating to skin in concentrations of 0.5 to 1.0% in alcohol. [51],[56],[22],[55]

**Toxicity:** Unknown.

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: 0.1 mg/kg in water [104]

Carcinogenicity: unknown

Mutagenicity: probable [58]

**Exposure:** Unknown



Chloroethane

 $C_2H_5Cl$ 

CAS RN: 75-00-3

Syn: Chloroethane \* Ethane, chloro- \* Aethylis \* Aethylis chloridum \*  
 Anodynon \* Chelen \* Chlorene \* Chlorethyl \* Chloridum \* Chloryl \* Chloryl  
 anesthetic \* Cloretilo \* Ether chloratus \* Ether hydrochloric \* Ether  
 muriatic \* Ethyl chloride \* Hydrochloric ether \* Kelene \* Monochlorethane \*  
 Monochloroethane \* Muriatic ether \* Narcotile \* NCI-C06224 \* UN 1037 (DOT)  
 \*

Molecular formula:  $CH_3CH_2Cl$ 

Monochlorinated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	64.5147	
Specific gravity:	0.8978	[105], [106]
	0.89600	[49]
Boiling point:	12.5°C	[22]
	12.4°C	[104]
	12.3°C	[10], [51], [106], [105]
	12.27°C	[49], [7]
	12.2°C	[107], [48], [32]
	12.°-13°C	[56]
Melting point:	-136.°C	[107]
	-136.4°C	[105], [49], [106]
	-138.°C	[10]
	-138.3°C	[104], [7]
	-138.7°C	[108], [48]
	-139.°C	[51], [32]
	-140.85°C	[22]
Refractive index:	1.3680	[49]
	1.3676	[105], [106]
Vapor pressure:	25.12 kPa @ -20°C	(188.41mm) [7]
	34.38 @ -13.48°C	(257.86mm) [105]
	44.88 @ -7.64°C	(336.61mm) [7]
	53.33 @ -3.9°C	(400mm) [105]
	57.62 @ -1.88°C	(432.19mm) [7]
	60.93 @ 0°C	(457mm) [104]
	71.86 @ 3.45°C	(539mm) [7]
	93.33 @ 10°C	(700mm) [104]
	106.71 @ 14°C	(800.4mm) [7]
	133.32 @ 20°C	(1000mm) [51], [104]
	135.03 @ 20.5°C	(1012.8mm) [7]
	141.8 @ 20°C	(1064mm) [32]
	159.88 @ 25°C	(1199.22mm) [49]
	192.5 @ 30°C	(1444mm) [104]
	202.6 @ 32.5°C	(1520mm) [105]
	295.87 @ 44.6°C	(2219.2mm) [7]
Vapor density:	2.23	[104]
	2.22	[51], [108], [7]
	2.2	[107], [32]
Evaporation rate:	>>1.	[32]

## 202 - Chloroethane

Relative dielectric permittivity:	12.7 @ -10°C	[11]
	10.65 @ 20°C	[11]
	10.36 @ 25°C	[11]
	9.45 @ 20°C	[49], [10]
	6.29 @ 170°C	[20]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.009288 W/(m-K)	[49]
Electrical resistivity:	>3.33 MOhm-m @ 0°C	[49], [11]
Critical temperature:	187.2°C [105], [107], [10], [108], [49], [22]	
Critical pressure:	5.3 MPa	[49], [22]
	5.269	[105], [10], [108]
	5.23	[107]
Dynamic viscosity:	0.392 mPa-s @ -20°C	[48]
	0.354 @ -10°C	[48]
	0.320 @ 0°C	[48]
	0.292 @ 5°C	[49], [7]
	0.291 @ 10°C	[48]
	0.279 @ 10°C	[49]
	0.278 @ 20°C	[47]
	0.244 @ 30°C	[48]
	0.234 @ 40°C	[47]
	0.224 @ 40°C	[48]
Kinematic viscosity:	0.426 $\mu\text{m}^2/\text{s}$ @ -20°C	
	0.385 @ -10°C	
	0.348 @ 0°C	
	0.325 @ 5°C	
	0.316 @ 10°C	
	0.311 @ 10°C	
	0.310 @ 20°C	
	0.265 @ 30°C	
	0.261 @ 40°C	
	0.243 @ 40°C	
Surface tension:	21.18 mN/m @ 5°C	[10]
	21.20 @ 5°C	[49], [7]
	20.58 @ 10°C	[10]
	20.64 @ 10°C	[49]
	19.5 @ 20°C	[107]
Contact angle:	unknown	
Thermal expansion coefficient:	0.0021 K <sup>-1</sup> @ 20°C	[49]
Compressibility:	unknown	
Vapor diffusion:	unknown	
Solution diffusion:	unknown	
Electric dipole moment:	6.838x10 <sup>-30</sup> C-m	[49], [105], [10]
Ionization potential:	10.97 eV (EI)	[105]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	4.455 kJ/mol	[107], [10], [105]
	4.452	[49]
Heat of vaporization:	26.4212 kJ/mol	[105]
	24.67	[10]
	24.652	[49]
	24.45	[107]
Heat of sublimation:	unknown	

Heat capacity @ 25°C:	0.1112 kJ/(mol-K)	(liq)	[108]
	0.1044	(liq)	[105]
	0.0628	(gas)	[105]
	0.0626	(gas)	[10]
	0.0624	(gas)	[108]
Heat of combustion:	-1350. kJ/mol @ 20°C	(liq)	[49]
	-1413.05	(gas)	[49]
	-1325.96 @ 20°C	(gas)	[105]
Heat of formation:	-136.62 kJ/mol @ 25°C	(liq)	[105]
	-136.52	(liq)	[49]
	-112.3	(gas)	[10]
	-112.26	(gas)	[49]
	-112.25	(gas)	[105]
Gibbs (free) energy:	-59.45 kJ/mol @ 25°C	(liq)	[105]
	-60.54	(gas)	[10]
	-60.50	(gas)	[105]
Analytical chemistry: pP <sub>oct</sub> =	1.54 (calculated)		[104], [8]
	1.49		[31]
	1.43		[21], [24]
pK <sub>s</sub> =	NA		
pK <sub>a</sub> =	NA		[31]
pK <sub>BH</sub> =	NA		
Henry's law constant =	1.48 kPa-m <sup>3</sup> /mol		[41]
	0.942		[41]
	0.859		[24]
	0.861 @ 25°C		[41]
Hydrolysis half-life =	3.3x10 <sup>6</sup> sec		[13], [8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Slightly soluble in water. Very soluble in ethanol. Miscible with ether. [51],[105],[22]

0.45 wt% in water @ 0°C	[10]
0.333 wt% in water @ 0°C	[104]
0.447 wt% in water @ 0°C	[49], [7]
0.57 wt% in water @ 20°C	[32]
0.574 wt% in water @ 20°C	[104], [108]
48.3 wt% in alcohol	[108]

Form: Colorless liquid or gas. Gas at room temperatures and pressures. Characteristic pungent, ether-like odor. Burning taste. Technical grades are 98-100% pure. Shipped in liquid form under pressure. [51],[108],[107],[104],[56],[7],[22],[32]

Use: Ethylating agent in the manufacture of tetraethyl lead, dyes, drugs, perfumes and ethyl cellulose; local or general anesthetic (freezing); refrigeration compound; solvent for fats oils, waxes, phosphorus, acetylene, and many resins; in organic synthesis of perchloroethane, esters, and Grignard reagents; propellant in aerosols; insecticides; alkylating agent. [108],[104],[56],[7],[22],[32]

## 204 - Chloroethane

**Fire and explosion hazard:** Very high.

Flash point: (CC) -50°C [32],[51],[107],[49],[22]

(OC) -42.78°C [107]

uel: 15.4% [32],[51]

12% [107]

14.8% [105]

lel: 3.8% [32],[51]

3.6% [107]

4% [105]

Autoign. temp.: 519°C [32],[51],[107],[22]

Extremely flammable liquid or gas. Highly volatile, extremely flammable gas at ordinary room temperature and pressure. Dangerous fire hazard when exposed to heat, flame, sparks or oxidizing materials. Burns with smoky, greenish flame. Dangerous explosion hazard, in the form of vapor, when exposed to heat or flame. Flashback along vapor trail may occur. Fire emits toxic gases and vapors such as hydrogen chloride, phosgene, and carbon monoxide. Reacts with water or steam to produce toxic and corrosive fumes. Fight fire with CO<sub>2</sub> or dry chemical, foam and stopping flow of gas. Cool exposed containers with water. For large fires it is best to let fire burn. [51],[108],[56],[32],[55]

**Incompatibility:** Chemically active metals such as sodium, potassium, calcium, powdered aluminum, zinc, and magnesium and their alloys. Can react vigorously with oxidizing materials. [51],[56],[32],[55]

**Handling:** Keep away from heat, sparks, open flame, sources of ignition, and light. Avoid breathing vapor using appropriate respirator or self-contained breathing apparatus. Use with adequate ventilation (fume hood). Prevent repeated or prolonged skin contact and any reasonable probability of eye contact (neoprene or rubber gloves and overclothing; chemical goggles). Remove wet or contaminated clothing immediately to avoid flammability hazard. Keep container tightly closed, out of sun, and away from heat. Store in cool, dry, well-ventilated, flammable liquid storage area or cabinet. Cylinder temperature should not exceed 52°C (125°F). [51],[107],[56],[32],[55]

**Health effects:** Chloroethane is a narcotic and toxic irritant. Routes of entry are inhalation of gas, percutaneous absorption, ingestion, and eye and skin contact. Points of attack include liver, kidneys, respiratory system, and cardiovascular system. Spilled on the skin, it may cause irritation and frostbite. Vapor or mist is irritating to the eyes, mucous membranes, and upper respiratory tract. Short-term exposure may cause drowsiness, unconsciousness, irregular heart beat, and death. Signs of overexposure may include abdominal cramps, vomiting, headache, cough, apparent inebriation, incoordination and dizziness. Long-term exposure may cause liver damage and accumulation of fat in the kidneys, cardiac muscles, and liver. It is the least toxic of all the chlorinated hydrocarbons. [51],[108],[107],[56],[7],[32],[55]

**Toxicity:** Very low.TWA: 1000 ppm (2600 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: 20000 ppm (52,500 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 3.7-4.5 ppm (10-12 mg/m<sup>3</sup>) -- recognition [104]

Carcinogenicity: unknown

Mutagenicity: unknown

**Exposure:****External:**Non-lethal: 40000 ppm (105.5 g/m<sup>3</sup>) -- eye irritation [32]

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: unknown

**Inhalation:**

Short-term Inhalation Limits: unknown

Non-lethal: 13000 ppm (34 g/m<sup>3</sup>) -- CNS effects [51]13000 ppm (34 g/m<sup>3</sup>) -- slight symptoms of poisoning [104]19000 ppm (50 g/m<sup>3</sup>) for 12 min -- weak analgesia [104]25000 ppm (66 g/m<sup>3</sup>) -- incoordination [7]33600 ppm (88 g/m<sup>3</sup>) for 30 sec -- toxic effect [104]33600 ppm (88 g/m<sup>3</sup>) (3.36% by vol.) for 5 min -- noisy  
talkativeness followed by incoordination. [104]40000 ppm (105.5 g/m<sup>3</sup>) -- dizziness, eye irritation, and  
abdominal cramps [7]

Lethal: unknown

## 206 - Chloroform

Chloroform

CHCl<sub>3</sub>

CAS RN: 67-66-3

Syn: Chloroform \* Methane, trichloro- \* Formyl trichloride \* Freon 20 \*  
 Methane trichloride \* Methenyl trichloride \* Methyl trichloride \* NCI-  
 C02686 \* R 20 \* R 20 (refrigerant) \* RCRA Waste Number U044 \* TCM \*  
 Trichloroform \* Trichloromethane \* UN 1888 (DOT) \*

Molecular formula: CHCl<sub>3</sub>

Polychlorinated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	119.378	
Specific gravity:	1.49845	[51]
	1.4985	[10]
	1.49	[107], [32]
	1.48911	[49]
	1.489	[104], [48]
	1.4832	[105]
Boiling point:	62.°C	[104]
	61.7°C	[10], [105]
	61.26°C	[51]
	61.2°C	[107], [48], [22]
	61.178°C	[49]
	61.°C	[32]
Melting point:	-63.5°C	[105], [51], [107], [10], [48], [22]
	-63.52°C	[49]
	-64.°C	[104]
Refractive index:	1.4486	[10]
	1.4459	[49], [105]
Vapor pressure:	4.633 kPa @ -10°C	(34.75mm) [41]
	5.333 @ -7.1°C	(40mm) [105]
	8.13 @ 0°C	(61mm) [41]
	13.33 @ 10.4°C	(100mm) [105], [51]
	21.33 @ 20°C	(160mm) [104], [108]
	25.97 @ 25°C	(194.8mm) [49]
	32.66 @ 30°C	(245mm) [104]
Vapor density:	4.12	[104], [51]
	4.1	[107], [32]
Evaporation rate:	11.6	[32]
	10.45	[49]
Relative dielectric permittivity:	6.67 @ -60°C	[105]
	6.12 @ -40°C	[105]
	6.34 @ -30°C	[2]
	5.61 @ -20°C	[105]
	6.12 @ -20°C	[2]
	5.98 @ -10°C	[2]
	5.93 @ 0°C	[2]
	4.930 @ 5°C	[2]
	5.86 @ 10°C	[2]
	4.85 @ 17°C (3 MHz)	[2]
	5.105 @ 17.5°C	[2]
	5.02 @ 20°C	[2]
	4.816 @ 20°C	[2]
	4.806 @ 20°C	[49], [105], [11]
	4.80 @ 20°C (1.8 MHz)	[2]

	4.72 @ 25°C (5 MHz)	[2]	
	4.67 @ 25°C (28 MHz)	[2]	
	4.719 @ 25°C (45 MHz)	[2]	
	4.641 @ 25°C	[11]	
	4.639 @ 25°C	[15]	
	4.665 @ 30°C	[2]	
	3.7 @ 100°C	[105], [11]	
	3.3 @ 140°C	[105]	
	2.9 @ 180°C	[105]	
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	0.121 W/(m-K) @ 12°C	[10], [48]	
	0.12104 @ 16°C	[105]	
	0.1030 @ 20°C	[105]	
	0.129 @ 20°C	[48]	
	0.138 @ 30°C	[48]	
Electrical resistivity:	>100. MOhm-m @ 25°C	[49]	
	>0.5 @ 25°C	[11], [10]	
Critical temperature:	263.4°C	[49], [10]	
	263.2°C	[107]	
	263.°C	[105]	
Critical pressure:	5.472 MPa	[105], [107], [10]	
	5.329	[49]	
Dynamic viscosity:	0.855 mPa-s @ -13°C	[105]	
	0.700 @ 0°C	[105], [48]	
	0.643 @ 8.1°C	[105]	
	0.63 @ 10°C	[48]	
	0.596 @ 15°C	[10], [105], [48]	
	0.580 @ 20°C	[105], [48]	
	0.542 @ 25°C	[48]	
	0.5357 @ 25°C	[49]	
	0.514 @ 30°C	[105], [48]	
	0.467 @ 40°C	[48]	
Kinematic viscosity:	0.576 $\mu\text{m}^2/\text{s}$ @ -13°C		
	0.472 @ 0°C		
	0.434 @ 8.1°C		
	0.423 @ 10°C		
	0.402 @ 15°C		
	0.391 @ 20°C		
	0.364 @ 25°C		
	0.3612 @ 25°C		
	0.347 @ 30°C		
	0.314 @ 40°C		
Surface tension:	27.14 mN/m @ 20°C air	[105]	
	27.16 @ 20°C	[49]	
	26.53 @ 25°C	[49]	
	25.25 @ 30°C	[49]	
	24.53 @ 40°C	[15]	
Contact angle: [18]			
	sessile	advancing	receding
quartz	8	11	8
calcite	14	21	5
biotite	8	11	9
Ca-mont.	7	swelled	swelled

## 208 - Chloroform

Thermal expansion coefficient:	0.00128 K <sup>-1</sup>	[48]
	0.00126	[49]
Compressibility:	0.855 nPa <sup>-1</sup> @ 0°C	[105]
	0.919 @ 10°C	[105]
	0.994 @ 20°C	[105]
	0.998 @ 20°C	[49]
	1.081 @ 30°C	[105]
	1.179 @ 40°C	[105]
Vapor diffusivity:	9.1 μm <sup>2</sup> /s @ 0°C	[47]
Solution diffusivity:	2.5 nm <sup>2</sup> /s in Benzene	[47]
	1.38 in Ethanol	[47]
Electric dipole moment:	3.836x10 <sup>-30</sup> C-m	[49]
	3.369x10 <sup>-30</sup>	[105], [10]
Ionization potential:	11.42 eV (PI)	[105]
Magnetic volume susceptibility:	-9.30x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	983. m/s @ 15°C	[105]
	987. @ 25°C	[105]
Heat of melting:	9.546 kJ/mol	[10]
	9.540	[49]
	8.8	[105], [107]
Heat of vaporization:	31.4031 kJ/mol	[105]
	29.64	[107], [10]
	29.37	[49]
Heat of sublimation:	31.32 kJ/mol	[10]
Heat capacity @ 25°C:	0.1155 kJ/(mol-K) (liq)	[105]
	0.11690 @ 30°C (liq)	[49]
	0.0657 (gas)	[105]
	0.0654	[10]
Heat of combustion:	-401.96 kJ/mol @ 25°C (liq)	[49]
	-373.5 @ 20°C (liq)	[105]
Heat of formation:	-132.3 kJ/mol @ 25°C (liq)	[10]
	-134.47 (liq)	[49]
	-102.93 (gas)	[49]
	-103.0 (gas)	[10]
Gibbs (free) energy:	-71.9 kJ/mol @ 25°C (liq)	[10]
	-70.17 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	1.97 @ 20°C	[104], [8], [21], [31]
	1.94	[21]
	1.90	[27]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	0.324 kPa-m <sup>3</sup> /mol @ 25°C	[41]
	0.737 @ 37°C	[41]
Hydrolysis half-life =	1.1x10 <sup>11</sup> sec	[13]
	3.9x10 <sup>7</sup> to 1.1x10 <sup>11</sup> sec	[8]

Electrochemical data: Wawzonek and Duty (1961), Meites and Zuman (1977), Meites et al. (1977a)

Clay-organic interaction data: [8][18]



**Solubility:** Slightly soluble in water. Soluble in acetone. Miscible with ethanol, ether, benzene, petroleum ether, carbon tetrachloride, carbon disulfide, ligroin, solvent naphtha, oils and most organic solvents. [105],[108],[22],[10]

1.0	wt% in water @ 15°C	[104]
0.82	wt% in water @ 20°C	[10]
0.80	wt% in water @ 20°C	[104],[32]
0.815	wt% in water @ 20°C	[49]
0.93	wt% in water @ 25°C	[104]

**Form:** Clear, colorless liquid. Characteristic ether-like odor. Sweet taste. Pure chloroform is light sensitive and reagent grade usually contains 0.5-1.0% (typically 0.75%) ethanol as stabilizer. [51],[107],[56],[108],[22]

**Use:** As a solvent for fats, oils, rubber, alkaloids, waxes, gutta-percha, resins; as cleansing agent; in fire extinguishers to lower the freezing temperature of carbon tetrachloride; anesthetic; fumigants; insecticides; manufacture of fluorocarbons for refrigerant propellants (Freon 22), fluorocarbon resins, artificial silk, floor polishes, plastics; general solvent in plastics, dyes, cleaning and dry cleaning industries; in chemical analysis and assays; in standard solutions as preservative and bactericide; electronic circuit manufacturing; extraction and purification of penicillin and other pharmaceuticals; primary source for chlorodifluoromethane. Chloroform is widely distributed in the atmosphere and water including most municipal drinking supplies. [104],[56],[5],[22],[32]

**Fire and explosion hazard:** Very low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Practically nonflammable liquid but very volatile. Very slight fire hazard if exposed to high heat. When heated to decomposition it emits toxic fumes of hydrochloric acid, hydrogen chloride, chlorine, phosgene and carbon monoxide. In the presence of air and light, it slowly reacts to form toxic phosgene, chlorine, carbon monoxide, carbon dioxide and hydrogen chloride gases. Stop discharge if possible. Use extinguishing media appropriate to surrounding fire conditions. [51],[107],[56],[32],[55]

**Incompatibility:** With strong caustics and chemically active metals such as aluminum, lithium, magnesium powder, sodium, or potassium; (acetone + a base), alkali, dinitrogen tetroxide, fluorine, potassium tert-butoxide, sodium, (sodium hydroxide + methanol), (potassium hydroxide + methanol), sodium methoxide, triisopropylphosphine, disilane, (perchloric acid + phosphorus pentoxide), sodium methylate, sodium hydroxide. [51],[56],[32]

**Handling:** Avoid heat and light. Very volatile so use in well-ventilated area (fume hood) with appropriate respirator or self-contained breathing apparatus. Prevent any reasonable probability of skin or eye contact (PVA synthetic latex, neoprene, leather, votin or nitrile gloves and overclothes; splash-proof chemical goggles). Remove non-impervious clothing promptly if contaminated. Keep container tightly closed. Store in secure poison area away from light and heat. [107],[56],[53],[32]

## 210 - Chloroform

**Health effects:** Chloroform is an anesthetic and suspected human carcinogen. Routes of entry are inhalation of vapors, ingestion, and skin and eye contact. Points of attack include liver, kidneys, heart, eyes, and skin. Inhalation causes dilation of the pupils with reduced reaction to light, as well as reduced intraocular pressure, headache, nausea, dizziness, drunkenness, narcosis. In the initial stages there is a feeling of warmth on the face and body, then an irritation of the mucous membranes and skin followed by nervous aberration. Prolonged inhalation will bring on paralysis accompanied by cardiac respiratory failure and finally death. Chronic effects of overexposure may include heart, liver and kidney damage, gastrointestinal effects, end embryotoxicity. It may produce burns if left in contact with the skin. Listed as a carcinogen by the EPA. [51],[107],[56],[5],[108],[22],[32],[55]

**Toxicity:** Moderate.

TWA: 10 ppm (50 mg/m<sup>3</sup>) -- suspected human carcinogen [1]

STEL no value set [1]

CL: 2 ppm (10 mg/m<sup>3</sup>) based on a 1 hr sample -- recommended standard [51],[56]

IDLH: 1000 ppm (4900 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 205-307 ppm (1000-1500 mg/m<sup>3</sup>) [107]

6-600 ppm (30-3000 mg/m<sup>3</sup>) -- detection [104]

4-1200 ppm (20-6000 mg/m<sup>3</sup>) -- recognition [104]

50-300 ppm -- with olfactory fatigue [32]

Carcinogenicity: suspected human carcinogen [1],[51],[56],[5]

Mutagenicity: experimental teratogen, neoplastic effects [51]  
nonmutagenic [30]

**Exposure:**

**External:**

Non-lethal: unknown

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: 140 mg/kg body wt -- death of an adult human [51]

0.5-5.0 g/kg [107]

546 mg/kg body wt -- death of an adult male [51]

**Inhalation:**

Short-term Inhalation Limits: 50 ppm (250 mg/m<sup>3</sup>) for 10 min [107]

Non-lethal: >50 ppm (250 mg/m<sup>3</sup>) -- unsatisfactory [104]

100-200 ppm chronic exposure -- enlarged liver [51]

205 ppm (1000 mg/m<sup>3</sup>)/1 yr -- liver and kidney damage [51]

500 ppm (2490 mg/m<sup>3</sup>) -- symptoms of illness [104]

1025 ppm (5000 mg/m<sup>3</sup>) for 7 min -- CNS effects [51]

>1000 ppm -- drowsiness, nausea, and headache [51]

2000 ppm for 60 min -- severe toxic effects [104]

2000-2500 ppm for several hours -- maximum tolerated [51]

14000 ppm (68 g/m<sup>3</sup>) for 30-60 min -- dangerous to life [51]

Lethal: 25000 ppm (122 g/m<sup>3</sup>) for 5 min [55]

Chloromethane

CH<sub>3</sub>Cl

CAS RN: 74-87-3

Syn: Chloromethane \* Methane, chloro- \* Artic \* Methyl chloride \*  
 Monochloromethane \* R 40 \* RCRA Waste Number U045 \* UN 1063 (DOT) \*

Molecular formula: CH<sub>3</sub>-Cl

Monochlorinated Aliphatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	50.4878	
Specific gravity:	0.9214	[49]
	0.92	[10], [22], [32]
	0.918	[51]
	0.9159	[105]
	0.991 @ -25°C	[104]
	0.997 @ -24°C	[107], [7]
Boiling point:	-23.7°C	[51], [22]
	-24. °C	[104]
	-24.2°C	[49], [105], [107], [32]
	-24.22°C	[10], [7]
Melting point:	-97. °C	[51]
	-97.5°C	[7]
	-97.6°C	[22], [32]
	-97.7°C	[49], [10], [107], [104]
	-97.73°C	[105]
Refractive index:	1.3389	[105]
	1.3384	[49]
	1.3661 @ -10°C	[105]
	1.3712 @ -23.7°C	[10], [22]
Vapor pressure:	506.6 kPa @ 20°C (3800mm)	[104]
	574.6 @ 25°C (4309.7mm)	[49], [23]
	678.87 @ 30°C (5092mm)	[104]
Vapor density:	1.8	[104], [32]
	1.785	[10]
	1.78	[51]
	1.7	[107]
Evaporation rate:	NA	
Relative dielectric permittivity:	12.6 @ -20°C	[105], [11]
	12.93 @ -25°C	[49]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.19247 W/(m-K) @ -15°C	[105]
Electrical resistivity:	NA	
Critical temperature:	143.8°C	[105]
	143.6°C	[107]
	143.1°C	[10], [49], [7]
Critical pressure:	6.68 MPa	[10], [49], [105], [107], [7]
Dynamic viscosity:	0.449 mPa-s @ 15°C	[105]
	0.393 @ 30°C	[105]
Kinematic viscosity:	0.490 μm <sup>2</sup> /s @ 15°C	
	0.429 @ 30°C	
Surface tension:	19.5 mN/m @ 0°C	[7]
	16.2 @ 20°C (air)	[105], [107]
Contact angle:	NA	
Thermal expansion coefficient:	0.00209 K <sup>-1</sup> @ -30° - 30°C	[49]

## 212 - Chloromethane

Compressibility:	unknown	
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	$6.238 \times 10^{-30}$ C-m	[105]
Ionization potential:	11.3 eV (PI,S)	[105]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	6.435 kJ/mol	[10]
	6.431	[49]
Heat of vaporization:	22.5053	[105]
	21.5495	[10]
	21.413 kJ/mol	[107]
	21.40	[49]
Heat of sublimation:	unknown	
Heat capacity @ 20°C:	0.803 kJ/(mol-K) (liq)	[49]
@ 25°C:	0.0408 (gas)	[10], [105]
Heat of combustion:	-764.01 kJ/mol @ 25°C (gas)	[49]
	-687.47 @ 20°C (gas)	[105]
Heat of formation:	-82.02 kJ/mol @ 25°C (gas)	[10]
	-81.965 (gas)	[49]
	-80.89 (gas)	[105]
Gibbs (free) energy:	-58.49 kJ/mol @ 25°C (gas)	[10]
	-57.44 (gas)	[105]
Analytical chemistry: $pP_{oct}$ =	0.95	[31]
	0.91	[8], [21]
	0.90	[41]
$pK_s$ =	NA	
$pK_a$ =	NA	[31]
$pK_{BH}$ =	NA	
Henry's law constant =	0.67 kPa-m <sup>3</sup> /mol	[41]
	0.0 @ 28°C	[41]
Hydrolysis half-life =	$2.9 \times 10^7$ sec	[13]
	$3.6 \times 10^7$ sec	[8]

Electrochemical data: Meites et al. (1977a).

Clay-organic interaction data: Unknown

Solubility: Slightly soluble in water. Soluble in ethanol. Miscible with benzene, chloroform, ether, glacial acetic acid, carbon tetrachloride. [51], [7], [22], [49], [10], [104]

0.648 wt% in water @ 30°C	[49]
0.48 wt% in water @ 25°C	[10]
4000. cm <sup>3</sup> /L water	[104]
280. cm <sup>3</sup> in 100 g water @ 16°C	[10]
3500. cm <sup>3</sup> in 100 g ethanol @ 20°C	[10]
4000. cm <sup>3</sup> in 100 g acetone	[10]

Form: Colorless gas. Odorless to faint, sweet, non-irritating ether-like odor. Sweet taste. Shipped as liquified gas. Commercial grades are approximately 99.5% pure. [51], [107], [56], [7], [22]

**Use:** Manufacturing of silicones, tetraethyl lead, methyl cellulose, fumigants and organic chemicals (methylene chloride, chloroform, carbon tetrachloride); refrigerant; low temperature solvent in the synthetic rubber industry; catalyst carrier in polymerization; medicine; fluid for thermometric or thermostatic equipment; methylating and chlorinating agent in organic chemistry; extractant; herbicide; propellant in polystyrene foam production; extractant for greases, oils and resins in petroleum refining; intermediate in drug manufacturing. Present in cigarette smoke (1200 ppm). [104],[56],[7],[22],[32]

**Fire and explosion hazard:** Very high.

Flash point: (CC) <0°C [107],[51]

(OC) <0°C [49]

UEL: 19% [32],[55]

17.2% [107],[51],[7]

11.4% [105]

LEL: 10.7% [105]

8.1% [107],[51],[7]

7.6% [32]

Autoign. temp.: 632.2°C [107],[51],[105]

Extremely flammable gas. Very dangerous fire hazard when exposed to heat, flame, or powerful oxidizers. Moderate explosion hazard when exposed to heat or flame. Flashback may occur along vapor trail. Containers may explode if heated. Emits highly toxic fumes of hydrogen chloride gas, phosgene gas, CO and CO<sub>2</sub> when heated to decomposition. Fight fire with dry chemical powder or CO<sub>2</sub>; water spray to knock down vapor. Stop flow of gas if possible. Cool exposed containers with water. [32],[107],[32],[55]

**Incompatibility:** Powdered Al; aluminum trichloride; ethylene; interhalogens; metals; galvanized iron. In the presence of catalytic amounts of aluminum chloride, powdered aluminum and chloromethane interact to form pyrophoric trimethylaluminum. Chloromethane may react explosively with: magnesium, zinc, potassium, and sodium or their alloys. [51],[107],[56],[32],[55]

**Handling:** Keep away from heat, sparks, open flame, sources of ignition. Ground storage cylinders and system before transferring liquid or gas. Avoid breathing vapor using appropriate respirator or self-contained breathing apparatus. Avoid eye or skin contact (leather or PVA gloves and over clothing; chemical goggles). WARNING: incompatible with natural rubber and many neoprene composites while polyvinyl alcohol is unaffected. Remove non-impervious clothing promptly if contaminated to avoid flammability hazard. Safety shower and eye bath should be provided. Use in well-ventilated area only (fume hood). Keep container tightly closed. Store in cool, dry, well-ventilated, flammable liquid storage area or cabinet. Cylinder temperature should not exceed 52°C (125°F). [107],[56],[7],[32],[55]

## 214 - Chloromethane

**Health effects:** Chloromethane is a narcotic and suspected human carcinogen. Routes of entry are inhalation and skin or eye contact. Points of attack include liver, kidneys, skin, bone marrow, cardiovascular system, and central nervous system. It has very slight irritant properties and may be inhaled without noticeable discomfort. It has a weak narcotic action. Symptoms of exposure to high concentrations may include dizziness, headache, weakness, drowsiness, incoordination, mental confusion, extreme nervousness, nausea and vomiting, abdominal pains, hiccoughs, diplopia and dimness of vision followed by delirium, convulsions and coma. Death is immediate but if exposure is not fatal, recover is slow with degenerative changes to the central nervous system common. Liver, kidneys, and bone marrow may also be affected. Symptoms of chronic exposure to low concentrations include fatigue, loss of appetite, muscular weakness, staggering gait, difficulty in speech, drowsiness, dimness of vision, and damage to the central nervous system and possibly to the liver, kidneys, bone marrow, and cardiovascular system. Repeated exposures to chloromethane are dangerous because it is eliminated very slowly from the body which converts chloromethane into hydrochloric acid and methanol. Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. [51],[107],[56],[7],[32],[55]

### **Toxicity:** Low.

TWA: 50 ppm (105 mg/m<sup>3</sup>) [1]

STEL: 100 ppm (210 mg/m<sup>3</sup>) [1]

CL: 200 ppm (420 mg/m<sup>3</sup>) [51],[56]

IDLH: 10000 ppm (20.65 g/m<sup>3</sup>) [107],[56]

Peak: 300 ppm (620 mg/m<sup>3</sup>) for 5 min duration in a 3-hr period [51],[56]

Odor threshold: 10 ppm (21 mg/m<sup>3</sup>) [32],[104]

Carcinogenicity: suspected or confirmed human carcinogen [1]

Mutagenicity: possible teratogen [55]  
mutagenic [30]

### **Exposure:**

#### **External:**

Non-lethal: unknown

Lethal: unknown

#### **Oral:**

Non-lethal: unknown

Lethal: unknown

#### **Inhalation:**

Short-term Inhalation Limits: 100 ppm (210 mg/m<sup>3</sup>) for 5 min [107]

Non-lethal: 15-195 ppm (31-403 mg/m<sup>3</sup>) -- no effects seen [104]

Lethal: 20000 ppm (41 g/m<sup>3</sup>) for 2 hr [55]

Chromium

Cr

CAS RN: 7440-47-3

Syn: Chromium \* Chrome \* Cr \*

Molecular formula: Cr

Element

**Physical properties:**

Relative molecular mass:	51.996	[105]
Specific gravity:	7.20	[32], [10]
	7.18-7.20	[105]
	7.14	[108]
	7.1	[22], [47]
Boiling point:	2682.°C	[10]
	2672.°C	[47], [105]
	2642.°C	[108]
	2640.°C	[32]
	2200.°C	[22]
Melting point:	1857.°C	[47], [10]
	1857. ± 20°C	[105]
	1900.°C	[108], [22]
Refractive index:	NA	
Vapor pressure:	essentially 0. kPa @ 20°C	[32]
	0.133 @ 1616°C	[47], [105]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	NA	
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	96.2 W/(m-K) @ 0°C	[105]
	93.9 @ 25.2°C	[105]
Electrical resistivity:	1.29x10 <sup>-13</sup> MOhm-m @ 0°C	[105]
	1.3x10 <sup>-13</sup> @ 22°C	[105]
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	1590.+/-50 mN/m @ 1950°C in vacuum	[105]
Contact angle:	NA	
Thermal expansion coefficient:	0.000006 K <sup>-1</sup> @ 25°C	[105]
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	6.764 eV (VUS)	[105]
Magnetic volume susceptibility:	180.0x10 <sup>-6</sup> SI units @ 0°C	[105]
Speed of sound:	unknown	
Heat of melting:	20.5 kJ/mol	[10]
	15.32	[105]
	14.6	[108]
Heat of vaporization:	342. kJ/mol	[108]
	339.7	[10]
Heat of sublimation:	397.7 kJ/mol	[10]

## 216 - Chromium

Heat capacity @ 25°C:	0.0239 kJ/(mol-K)	(sol)	[105]
	0.02345	(sol)	[10]
	0.0234	(sol)	[108]
	0.02345	(liq)	[10]
	0.02080	(gas)	[10]

Heat of combustion: unknown

Heat of formation:	0.0 kJ/mol @ 25°C	(sol)	[105], [10]
	26.12	(liq)	[10]
	397.7	(gas)	[10]
	337.0	(gas)	[105]
Gibbs (free) energy:	0.0 kJ/mol @ 25°C	(sol)	[105], [10]
	22.36	(liq)	[10]
	292.2	(gas)	[105]
	174.3	(gas)	[10]

Analytical chemistry: pP<sub>oct</sub> = NA  
pK<sub>s</sub> = NA  
pK<sub>a</sub> = NA  
pK<sub>BH</sub> = NA  
Henry's law constant = NA  
Hydrolysis half-life = NA

Electrochemical data: Niki et al.(1986)

Clay-organic interaction data: inorganic

Solubility: Insoluble in water, HNO<sub>3</sub>. Soluble in dilute H<sub>2</sub>SO<sub>4</sub>, HCl.  
[22], [32], [47], [105], [108], [10]

Form: Steel-gray, lustrous metal available as lumps, granules, or powder. Very hard, but brittle, and extremely resistant to corrosion and oxidation. It has atomic number 24 (Group VIB) and valences of -2 to 6 (2, 3 and 6 are most common). Elemental chromium does not occur in nature. The principal ore is chromite (FeCr<sub>2</sub>O<sub>4</sub>). [105], [22], [54]

Use: It is used to harden steel, to manufacture stainless steel (chrome-steel or chrome-nickel-steel) and other alloys, in plating, to give glass an emerald green color, in nuclear and high-temperature research, in photographic fixing baths, in tanning leather, as a fuel additive and propellant additive, in the textile industry in dyeing, silk treating, printing, and moth-proofing wool, and as a catalyst for halogenation, alkylation, and catalytic cracking of hydrocarbons. The man-made <sup>51</sup>CR isotope is used as a tracer in various blood diseases and in the determination of blood volume. [105], [108], [22], [32], [54]

Fire and explosion hazard: Low

Flash point: NA

uel: NA

lel: 230 g/m<sup>3</sup> of metal dust [32]

Autoign. temp.: 400°C (layer) [32]

580°C (cloud) [32]



Nonflammable solid. Flammable solid in the form of dust or powder. Powder will explode spontaneously in air. Metal in contact with strong oxidizers may cause fire and explosions. Fight fire with dry sand, dry dolomite, dry graphite. Use extinguishing media appropriate to surrounding fire conditions. [105],[32],[55]

**Incompatibility:** Strong acids; strong oxidizing agents. [105],[56],[55]

**Handling:** WARNING: avoid all contact. Keep away from heat and open flame if in the form of dust or powder. Do not breathe vapor, dust or powder (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (chemical resistant gloves and suit; safety goggles or face shield). Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [55],[56],[32]

**Health effects:** Chromium compounds can act as allergens which cause dermatitis to exposed skin. Chromic acid has a corrosive effect on the skin and the mucous membranes of the upper respiratory tract. Chromium compounds in the +3 valence state are of a low order of toxicity. Compounds in the +6 state are irritants and corrosive. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include the respiratory system and lungs for chromium metal and insoluble salts; skin for soluble chromic and chromous salts; blood, lungs, respiratory system, liver, kidneys, eyes, and skin for chromic acid and chromates. Acute exposure to dust or mist may cause coughing and wheezing, headache, dyspnea, pain on deep inspiration, fever and loss of weight. Other symptoms include lacrimation, inflammation of the conjunctiva, nasal itch and soreness, epistaxis, ulceration and perforation of the nasal septum, congested nasal mucosa and turbinates, chronic asthmatic bronchitis, dermatitis and ulceration of the skin, inflammation of laryngeal mucosa, cutaneous discoloration, and dental erosion. [56],[108],[32],[54],[77],104]

**Toxicity:** Moderate.

TWA: 0.24 ppm (0.5 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

**Carcinogenicity:** Chromate salts are experimental and human carcinogens of the lungs, nasal cavity, and paranasal sinus; also an experimental carcinogen of the stomach and larynx. [105],[54]

**Mutagenicity:** equivocal tumorigenic agent by RTECS criteria [55]

**Exposure:** Unknown

## 218 - Chrysene

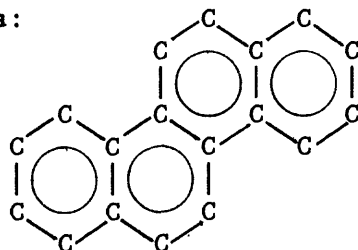
Chrysene

 $C_{18}H_{12}$ 

CAS RN: 218-01-9

Syn: Chrysene \* 1,2-Benzophenanthrene \* Benzo(a)phenanthrene \* 1,2-Benzphenanthrene \* Benz(a)phenanthrene \* CH \* CR \* 1,2,5,6-Dibenzonaphthalene \* RCRA Waste Number U050 \*

Structural formula:



Polynuclear Aromatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	228.293	
Specific gravity:	1.274	[10], [104], [105], [22], [108], [106]
Boiling point:	448.°C	[105], [22], [108], [10], [106]
Melting point:	254.°C	[104], [22], [108]
	255.°-256°C	[105], [106]
	253.°-254°C	[10]
Refractive index:	unknown	
Vapor pressure:	8.4x10 <sup>-8</sup> kPa @ 20°C (6.3x10 <sup>-7</sup> mm)	[41]
	8.4x10 <sup>-10</sup> kPa @ 25°C (6.3x10 <sup>-9</sup> mm)	[31]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	4.6 μm <sup>2</sup> /s	[59]
Solution diffusivity:	0.5 nm <sup>2</sup> /s in water	[59]
Electric dipole moment:	unknown	
Ionization potential:	7.85 eV	[41]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	26.15 kJ/mol	[105]
Heat of vaporization:	unknown	
Heat of sublimation:	117.6 kJ/mol	[10]
Heat capacity @ 25°C:	unknown	
Heat of combustion:	-8956.0 kJ/mol @ 20°C (sol)	[105]
Heat of formation:	145.3 kJ/mol @ 25°C (sol)	[10]
Gibbs (free) energy:	396.2 kJ/mol (gas)	[59]

Analytical chemistry:	pP <sub>oct</sub> =	5.61	[8],[31]
		5.91	[41]
	pK <sub>s</sub> =	NA	
	pK <sub>a</sub> =	>15.	[59]
		NA	[31]
	pK <sub>BH</sub> =	NA	
Henry's law constant =		7.36x10 <sup>-18</sup> kPa·m <sup>3</sup> /mol (calc)	[41]
		0.0039 dimensionless (calc)	[59]
Hydrolysis half-life =		NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

**Solubility:** Practically insoluble in water. Slightly soluble in ethanol, ether, acetone, benzene, carbon disulfide, glacial acetic acid. Soluble in hot benzene, hot toluene. [105],[22],[108]

0.00000015 wt% in water @ 15°C	[104]
0.0000006 wt% in water at 25°C	[104]
0.001-0.05 ppm in seawater @ 22°C	[104]
0.1 wt% in absolute alcohol @ 16°C	[10]
1. g/1300 mL absolute alcohol @ 25°C	
	[108]
1. g/480 mL toluene @ 25°C	[108]
5. vol% in toluene @ 100°C	[108]

**Form:** Colorless to red, off-white, or blue flakes or rhombic plates or crystals. [51], [104],[108],[10],[106],[55]

**Use:** Chrysene is a polynuclear aromatic hydrocarbon (PAH). PAHs are formed in any hydrocarbon combustion process and may be released from oil spills. The less efficient the combustion, the higher the PAH emission factor. It is a natural constituent of coal tar and present in automotive gasoline (0.23-6.7 mg/kg), gasoline engine exhaust (27-318 µg/m<sup>3</sup>), fresh motor oil (0.56 mg/kg) and used motor oil (86.2-236.6 mg/kg), bitumen (1.64-5.14 ppm), crude oil (6.9-17.5 ppm) and cigarette smoke (6.0 µg/100 cigarettes). [104],[56]

**Fire and explosion hazard:** Unknown

Flash point: unknown

uel: unknown

lel: unknown

Autoign. temp.: unknown

No information concerning flammability was found. Chrysene is probably not flammable. It may emit acrid smoke and irritating fumes, including CO and CO<sub>2</sub>, when heated to decomposition. Fight fire with water spray, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [51],[55]

**Incompatibility:** Strong oxidizing agents. [55]

## 220 - Chrysene

**Handling:** Avoid all contact. Prevent any reasonable possibility of skin or eye contact, or inhalation of dust or fumes (appropriate respirator or self-contained breathing apparatus, chemical resistant gloves, safety goggles, other protective clothing). Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [56]

**Health effects:** Chrysene is a suspected human carcinogen. Routes of entry include inhalation, ingestion, skin absorption, and eye and skin contact. Exposure may cause irritation. Harmful effects to humans have not been well studied. Test animals have formed carcinomas in stomach, lungs, breast and skin after exposure to relatively high levels. [56],[5],[55],[89]

**Toxicity:** Moderate

TWA: no value set -- suspected human carcinogen [1]

STEL: no value set

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: suspected human carcinogen [1],[104],[56]

animal limited evidence (IARC cancer review) [55]

Mutagenicity: positive mutagenicity in *Salmonella* test [104]

**Exposure:** Unknown

## Copper

Cu

CAS RN: 7440-50-8

Syn: Copper \* Cu \* Allbri natural copper \* Anac 110 \* Arwood copper \* Bronze powder \* CDA 101 \* CDA 102 \* CDA 110 \* CDA 122 \* C.I. 77400 \* C.I. Pigment metal 2 \* Copper-airborne \* Copper bronze \* Copper M 1 \* Copper-milled \* Copper powder \* Copper slag-airborne \* Copper slag-milled \* CuEP \* CuEPP \* Cu M2 \* Cu M3 \* DCuPl \* E-Copper \* E-Cu57 \* E-Cu F20GB \* 1721 Gold \* Gold bronze \* Kafar copper \* M 1 \* M 3 \* M 4 \* M1 (copper) \* M2 (copper) \* M3 (copper) \* M4 (copper) \* M3R \* M3S \* OFHC Cu \* Raney copper \*

Molecular formula: Cu

Element

## Physical properties:

Relative molecular mass:	63.546	[105]
Specific gravity:	8.96	[22], [105]
	8.92	[47], [51], [105], [10]
Boiling point:	2595.°C	[108], [22]
	2575.°C	[10]
	2567.°C	[47], [105]
	2324.°C	[51]
Melting point:	1084.5°C	[10]
	1083.4° ± 0.2°C	[105]
	1083.°C	[47], [51], [108], [22]
Refractive index:	NA	
Vapor pressure:	0.133 kPa @ 1628°C (1mm)	[51], [105]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	NA	
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	403. W/(m-K) @ 0°C	[105]
	401. @ 25°C	[105]
	398. @ 25°C	[105]
	385. @ 0°-100°C	[10]
Electrical resistivity:	1.534x10 <sup>-14</sup> MOhm-m @ 0°C	[105]
	1.678x10 <sup>-14</sup> @ 20°C	[105]
	1.7x10 <sup>-14</sup> @ 22°C	[105], [45]
	1.673x10 <sup>-14</sup>	[108]
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	1360. mN/m @ 1084°C	[105]
	1103. @ 1131°C	[20]
Contact angle:	NA	
Thermal expansion coefficient:	0.0000166 K <sup>-1</sup> @ 25°C	[105]
Compressibility:	NA	
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	NA	
Ionization potential:	7.724 eV (VUS)	[105]
Magnetic volume susceptibility:	-68.6x10 <sup>-6</sup> SI units @ 22.8°C	[105]

## 222 - Copper

Speed of sound:	4760. m/s long. wave in bulk annealed	[105]
	2325. shear wave in bulk annealed	[105]
	3810. long. wave in thin rod annealed	[105]
	5010. long. wave in bulk rolled	[105]
	2270. shear wave in bulk rolled	[105]
	3750. long. wave in thin rod rolled	[105]
Heat of melting:	13.27 kJ/mol	[10]
	13.02	[105], [108]
Heat of vaporization:	306.0 kJ/mol	[108]
	304.5	[10]
Heat of sublimation:	339.1 kJ/mol	[10]
Heat capacity @ 25°C:	0.0245 kJ/(mol-K) (sol)	[105], [10]
	0.0208 (gas)	[10]
Heat of combustion:	unknown	
Heat of formation:	0.0 kJ/mol @ 25°C (liq)	[105], [10]
	341.3 (gas)	[105]
	338.5 (gas)	[10]
Gibbs (free) energy:	0.0 kJ/mol @ 25°C (sol)	[105], [10]
	301.6 (gas)	[105]
	298.8 (gas)	[10]
Analytical chemistry:	pP <sub>oct</sub> =	NA
	pK <sub>s</sub> =	NA
	pK <sub>a</sub> =	NA
	pK <sub>BH</sub> =	NA
	Henry's law constant =	NA
	Hydrolysis half-life =	NA

Electrochemical data: Bertocci and Turner (1974)

Clay-organic interaction data: inorganic

**Solubility:** Insoluble in water. Very slightly soluble in HCl, NH<sub>4</sub>OH, ammonia water. Soluble in HNO<sub>3</sub>, hot H<sub>2</sub>SO<sub>4</sub>. [47], [105], [108], [22], [10]

**Form:** Reddish metal that can take on a bright metallic luster but turns dull when exposed to air. Available in the form of ingots, sheets, rod, wire, tubing, shot, or powder, and as single crystals or whiskers in high purity form. It is malleable, ductile, and a good conductor of heat and electricity (Mohs hardness of 3.0). It has atomic number 29 (Group IB), a valence of 1 or 2, and face-centered cubic structure. Cu can be found in its native state and also occurs in combined form in many minerals including chalcopyrite, chalcocite, and bornite. Commercially available high purity forms are 99.999% Cu. [51], [105], [108], [22]

**Use:** Copper is used in the manufacture of brass and bronze and other Cu alloys and for electrical conductors, ammunition, plumbing pipes, copper salts, works of art and coins. The sulfate is used in agricultural poisoning and as an algicide in water purification. [105], [108], [56], [54], [22]

**Fire and explosion hazard:** Low.

Flash point: NA

UEL: NA

LEL: NA

Autoign. temp.: NA

Nonflammable solid. Flammable in the form of dusts or mists. Fight fire with dry chemical powder. Do not use water. [22],[55]

**Incompatibility:** Strong acids; strong oxidizing agents; acid chlorides; halogens; ( $\text{Cl}_2 + \text{OF}_2$ ); 1-bromo-2-propyne. Magnesium metal is incompatible with Cu dusts and mists. WARNING: violent reaction may occur with acetylene, ammonium nitrate, bromates, chlorates, iodates, chlorine, chlorine trifluoride, ethylene oxide, fluorine, hydrogen peroxide, hydrazine mononitrate, hydrogen sulfide, hydrazoic acid, lead azide, potassium peroxide, sodium azide, and sodium peroxide. Reaction of copper wool, trichloroacetic acid in dimethyl sulfoxide is very exothermic. [51],[56],[55]

**Handling:** Keep away from heat and open flame when in the form of dust or powder. Do not breathe vapor, dust or powder (appropriate respirator or self-contained breathing apparatus required). Do not get in eyes, on skin, or on clothing (chemical resistant gloves and suit; safety goggles or face shield). Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. Air sensitive; store under nitrogen. [55],[56],[32]

**Health effects:** Copper metal is generally not toxic, but Cu can be toxic in the form of dust or fumes. Many copper compounds are hazardous substances. Routes of entry are inhalation of dust or fume, ingestion, and skin or eye contact. Points of attack include respiratory system, lungs, skin, liver, kidneys for dust and mists, and respiratory system, skin, eye, and risk of Wilson's disease for fumes. Inhalation of copper dust by animals has resulted in hemolysis of the red blood cells, deposition of hemofuscin in the liver and pancreas, and injury to the lung cells. Injection of the dust caused cirrhosis of the liver and pancreas. Copper salts act as irritant to human skin causing itching, erythema, and dermatitis. In the eyes, copper salts may cause conjunctivitis and even ulceration and turbidity of the cornea. The fumes and dust may cause upper respiratory tract irritation, metallic taste in the mouth, nausea, metal fume fever, and sometimes discoloration of the skin and hair. Drinking water supplied by copper pipes can cause cirrhosis and even death in infants but does not seriously affect older children and adults. [51],[56],[54],[32],[42]

## 224 - Copper

### Toxicity: Low.

TWA: 0.08 ppm (0.2 mg/m<sup>3</sup>) -- fumes [1]

0.38 ppm (1.0 mg/m<sup>3</sup>) -- dusts and mists [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: There is an excess of cancer cases in the Cu smelting industry. [51]

Mutagenicity: equivocal tumorigenic agent by RTECS criteria [55]

### Exposure:

#### External:

Non-lethal unknown

Lethal: unknown

#### Oral:

Non-lethal: 120 µg/kg body wt -- gastrointestinal tract effects [51]

Lethal: 2154 µg/g dry wt -- death of 13 month old infant [42]

#### Inhalation:

Short-term Inhalation Limit: unknown

Non-lethal: unknown

Lethal: unknown



o-Cresol

C<sub>7</sub>H<sub>8</sub>O

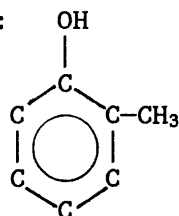
CAS RN: 95-48-7

Syn: o-Cresol \* Phenol, 2-methyl- \* 2-cresol \* o-Cresylic acid \* 1-Hydroxy-2-methylbenzene \* 2-Hydroxytoluene \* o-Hydroxytoluene \* o-Kresol \* 2-Methylbenzenol \* 2-Methylphenol \* o-Methylphenol \* o-Methylphenylol \* ortho-Cresol \* o-Oxytoluene \* RCRA Waste Number U052 \* o-Toluol \* UN 2076 (DOT) \*

Molecular formula: o-CH<sub>3</sub>-C<sub>6</sub>H<sub>4</sub>-OH

Monohydric Phenol

Structural formula:



## Physical properties:

Relative molecular mass:	108.14	
Specific gravity:	1.05	[107]
	1.047	[10], [51]
	1.041	[104]
	1.02734	[105]
	1.0273	[106]
	1.0460 (supercooled liquid)	[49]
Boiling point:	191.004°C	[49]
	191.°C	[104], [107], [106]
	190.95°C	[105]
	190.8°C	[10], [51]
Melting point:	31.°C	[104], [107]
	30.944°C	[49]
	30.94°C	[105]
	30.9°C	[10], [106]
	30.8°C	[51]
Refractive index:	1.5467	[49]
	1.5361	[10], [105], [106]
	1.5336 @ 46°C	[10]
Vapor pressure:	0.032 kPa @ 25°C (0.24mm)	[104]
	0.041 @ 25°C (0.31mm)	[49], [23]
	0.1333 @ 38.2°C (1mm)	[105], [51]
	0.6666 @ 64°C (5mm)	[104]
Vapor density:	3.72	[107], [51]
	3.7	[104]
Evaporation rate:	unknown	
Relative dielectric permittivity:	12.29 @ 25°C	[2]
	11.5 @ 25°C	[49], [105], [10], [11]
	6.31 @ 40°C	[49]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	7.69 MOhm-m @ 20°C	[11]
	7.87 @ 25°C	[49]
	23.3 @ 50°C	[49]
Critical temperature:	424.4°C	[49], [105], [10], [107]

## 226 - o-Cresol

Critical pressure:	5.01 MPa	[49],[105],[10],[107]
Dynamic viscosity:	4.49 mPa-s @ 40°C	[105]
	3.506 @ 46°C	[10]
Kinematic viscosity:	4.37 $\mu\text{m}^2/\text{s}$ @ 40°C	
	3.427 @ 46°C	
Surface tension:	40.3 mN/m @ 20°C	[107]
	34.8 @ 40.3°C	[49]
	21.5 @ 176°C	[49]
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	7.5 $\mu\text{m}^2/\text{s}$ (calc)	[59]
Solution diffusivity:	0.76 $\text{nm}^2/\text{s}$ (calc)	[59]
Electric dipole moment:	4.70x10 <sup>-30</sup> C-m	[10]
	5.47x10 <sup>-30</sup>	[49]
Ionization potential:	8.98 eV	[41]
Magnetic volume susceptibility:	-8.87x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	15.820 kJ/mol	[49]
	13.940	[105]
Heat of vaporization:	52.2818 kJ/mol	[105]
	45.191 (bp)	[49]
	44.9	[107]
	42.71	[10]
	64.39 @ 25°C	[49]
Heat of sublimation:	76.07 kJ/mol (fp)	[49],[10]
Heat capacity @ 25°C:	0.15456 kJ/ (mol-K) (sol)	[49]
	0.1304 (gas)	[10]
@ 31.05°C:	0.23292 (liq)	[49]
Heat of combustion:	-3695.7 kJ/mol @ 25°C (sol)	[105]
	-3693.30 (sol)	[49]
	-3514. (sol)	[107]
	-3695.3 @ 20°C (liq)	[105]
Heat of formation:	-204.60 kJ/mol @ 25°C (sol)	[49]
	-128.7 (gas)	[10]
	-128.574 (gas)	[49]
Gibbs (free) energy:	-37.10 kJ/mol @ 25°C (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	2.04	[21]
	1.95	[23],[21],[67],[59]
pK <sub>s</sub> =	unknown	
pK <sub>a</sub> =	10.26 in water @ 25°C	[10]
	10.287 in water @ 25°C	[49],[23]
	10.2 in water @ 25°C	[105],[11]
pK <sub>BH</sub> =	unknown	
Henry's law constant =	0.000047 dimensionless (calc)	[59]
Hydrolysis half-life =	unknown	

Electrochemical data: Meites and Zuman (1977)

Clay-organic interaction data: Erickson (1948), Greene-Kelly (1955).

**Solubility:** Slightly soluble in water. Soluble in glycol, dilute alkalis, and ordinary organic solvents. Very soluble in ethanol, ether, glycol, dilute alkalis. Miscible with ethanol @ 30°C, ether @ 30°C, acetone, benzene, chloroform, carbon tetrachloride. [05],[56],[14],[10],[104],[49]  
3.1 wt% in water @ 40°C [10],[104]  
3.08 wt% in water @ 40°C [49]  
5.6 wt% in water @ 100°C [104]

**Form:** Colorless to yellow crystals or liquid, darkening with exposure to air and light. Sweet tarry, phenolic-like odor. Some commercial preparations are 80-98% pure containing 2-20% phenol. Others are 99.2% pure with 0.2% phenol and 0.6% meta and para isomers. [51],[107],[104]

**Use:** Disinfectant; ore flotation agent; manufacture of chemicals (tricresylphosphate, coumarin, salicylaldehyde, cresylic acid), dyes, plastics, resins, perfumes, herbicides, and food antioxidants; textile scouring agent; surfactant. It occurs naturally as a constituent in coal, petroleum, wood, and natural runoff. It is present in automobile exhaust (0.5-1.0 ppm), roadway and asphalt runoff, and domestic sewage, and as a result of the general use of plastics, petroleum distillates, fuels, perfumes, oils, lubricants, metal cleaning and scouring compounds, and laboratory chemicals. [104],[56]

**Fire and explosion hazard: Moderate**

Flash point: (CC) 81.1°C [107],[51],[49]

uel: unknown

1e1: 1.4% @ 149°C [51]

1.35% [107]

Autoign. temp.: 599°C [107],[51]

Flammable solid or liquid. Moderate fire hazard when exposed to heat or flame. Slight explosion hazard in the form of vapor when exposed to heat or flame. Vapors form explosive mixtures with air. Emits highly toxic fumes of CO and CO<sub>2</sub> when heated to decomposition. Fight fire with water to blanket fire, CO<sub>2</sub>, dry chemical, foam, water spray. Stop discharge if possible. [51],[107],[55]

**Incompatibility:** Oxidizing agents; bases; light sensitive; air sensitive. Reacts violently with HNO<sub>3</sub>, oleum, chlorosulfonic acid. [51],[56],[55]

**Handling:** Avoid heat, flame, sparks, and sources of ignition. Prevent inhalation of vapors (appropriate respirator or self-contained breathing apparatus). Prevent any possibility of skin or eye contact (neoprene, nitrile or rubber overclothing and gloves; chemical goggles or faceshield (8-inch minimum)). Remove nonimpervious clothing promptly if wet or contaminated. Facilities for eye wash and quick body drenching should be available. Keep container tightly closed. Store in cool, dry, well-ventilated, flammable liquid storage area or cabinet away from light. Store in secure poison area. [107],[53],[56]

## 228 - o-Cresol

**Health effects:** o-Cresol is corrosive and a poison. Routes of entry are inhalation or percutaneous absorption of liquid or vapor, ingestion, and eye and skin contact. Points of attack include respiratory system, skin and eyes, kidneys, liver, and central nervous system. It is similar to phenol in its effect on the body but less severe. It has a corrosive action on the skin and mucous membranes and can produce severe burns after a few minutes contact and skin rash or dermatitis after repeated exposure. Gangrene may occur later. If it contacts the eyes, extensive damage and blindness may occur. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. Systemic poisoning has rarely been reported. Symptoms of systemic effects may develop in 20 to 30 minutes and include headache, dimness of vision, ringing in the ears, rapid breathing, CNS depression, muscular weakness, convulsions, mental confusion, and sometimes death. Signs of chronic poisoning include vomiting, difficulty in swallowing, salivation, diarrhea, loss of appetite, headache, fainting, dizziness, mental disturbances, and skin rash. If there has been severe damage to the liver and kidneys death may result. [51],[107],[56],[55],[67]

**Toxicity:** High.

TWA: 5 ppm (22 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 250 ppm (1105 mg/m<sup>3</sup>) [107]

Peak: unknown

Odor threshold: 0.26 ppm (1.14 mg/m<sup>3</sup>) [107]

0.0005-0.5 ppm (0.0002-2.2 mg/m<sup>3</sup>) [104]

0.09-0.65 ppm (0.4-2.9 mg/m<sup>3</sup>) in water [104]

0.65 ppm (2.9 mg/m<sup>3</sup>) in water [107]

Carcinogenicity: unknown

Mutagenicity: some evidence of neoplastic effects and tumor promotion  
[51],[107]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: 10 ppm (44 mg/m<sup>3</sup>) [107]

Non-lethal: unknown

Lethal: unknown

Cyclohexane

C<sub>6</sub>H<sub>12</sub>

CAS RN: 110-82-7

Syn: Cyclohexane \* Benzene hexahydride \* Hexahydrobenzene \* Hexamethylene  
 \* Hexanaphthene \*

Molecular formula: (CH<sub>2</sub>)<sub>6</sub>

Saturated Aliphatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	84.16128	
Specific gravity:	0.779	[104],[22],[107],[47]
	0.7786	[10]
	0.77855	[105],[49],[106]
Boiling point:	80.8°C	[48]
	80.74°C	[105],[10],[22],[107],[106]
	80.73°C	[49]
Melting point:	6.72°C	[49]
	6.55°C	[105],[107],[47],[106]
	6.5°C	[10]
	6.4°C	[48]
	6.3°C	[104],[22]
Refractive index:	1.42662	[105],[106]
	1.42623	[49],[10],[22]
Vapor pressure:	0.133 kPa @ -45.3°C (1mm)	[20],[47]
	5.33 @ 6.7°C (40mm)	[20],[47]
	10.3 @ 20°C (77mm)	[104]
	12.7 @ 20°C (95mm)	[32]
	13.04 @ 25°C (97.81mm)	[49]
	16.0 @ 30°C (120mm)	[104]
Vapor density:	2.98	[32]
	2.90	[104],[107],[51]
Evaporation rate:	2.6	[3]
Relative dielectric permittivity:	2.023 @ 20°C	[105],[10],[11]
	2.02431 @ 20°C	[49]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	1.43x10 <sup>9</sup> MOhm-m @ 25°C	[49]
Critical temperature:	280.49°C	[49]
	280.3°C	[10],[107]
	281.1°C	[20],[47]
Critical pressure:	4.075 MPa	[49]
	4.073	[10],[107]
	4.094	[47]
	4.111	[20]
Dynamic viscosity:	1.02 mPa-s @ 17°C	[105]
	0.975 @ 20°C	[49]
	0.980 @ 20°C	[10]
	0.898 @ 25°C	[49]
	0.820 @ 30°C	[49]
Kinematic viscosity:	1.31 μm <sup>2</sup> /s @ 17°C	
	1.25 @ 20°C	
	1.15 @ 25°C	
	1.05 @ 30°C	

## 230 - Cyclohexane

Surface tension:	26.432 mN/m @ 10°C	[10]
([10] values are calculated)	27.62 @ 20°C	[10]
	24.6 @ 20°C	[107]
	25.24 @ 20°C	[49]
	24.65 @ 25°C	[49]
	23.74 @ 30°C	[49]
	22.868 @ 40°C	[10]
	21.680 @ 50°C	[10]
	20.492 @ 60°C	[10]
	19.304 @ 70°C	[10]
	18.116 @ 80°C	[10]

Contact angle: [18]

	sessile	advancing	receding
quartz	9	12	8
calcite	9	12	9
biotite	7	10	7
Ca-mont.	7	10	9

Thermal expansion coefficient:	0.001220 K <sup>-1</sup>	[49]
Compressibility:	0.988 nPa <sup>-1</sup> @ 10°C	[105]
	1.110 @ 25°C	[105]
	1.140 @ 25°C	[49]
	1.202 @ 35°C	[105]
	1.256 @ 40°C	[105]
	1.314 @ 45°C	[105]
	1.435 @ 55°C	[105]
	1.488 @ 60°C	[105]
	1.784 @ 75°C	[105]
Vapor diffusivity:	8.6 lm <sup>2</sup> /s @ 45°C in air	[47]
	7.4 @ 15°C in O <sub>2</sub>	[47]
	7.6 @ 15°C in N <sub>2</sub>	[47]
	31.9 @ 15°C in H <sub>2</sub>	[47]

Solution diffusivity:	unknown	
Electric dipole moment:	0.	[10]
Ionization potential:	9.8 eV (PI,PE)	[105]
Magnetic volume susceptibility:	-7.879x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	2.6796 kJ/mol	[10]
	2.6773	[49]
	2.630	[105], [107]
	2.6074	[48]
Heat of vaporization:	29.977 kJ/mol	[10], [107]
	30.05	[49]
	30.303	[48]
	32.786	[105]
Heat of sublimation:	33.059 kJ/mol	[10]
Heat capacity @ 25°C:	0.1524 kJ/(mol-K) (liq)	[105]
	0.1063 (gas)	[105], [10], [49]
	0.157 (liq)	[10]
	0.156 (liq)	[49]
Heat of combustion:	-3922.5 kJ/mol @ 25°C (liq)	[105], [20]
	-3919.86 (liq)	[49]
	-3955.6 (gas)	[20]

Heat of formation:	-156.34	kJ/mol @ 25°C	(liq)	[10]
	-123.22		(gas)	[10]
	-156.29		(liq)	[20]
	-123.16		(gas)	[20]
	-156.19		(liq)	[49]
Gibbs (free) energy:	26.67	kJ/mol @ 25°C	(liq)	[10]
	31.78		(gas)	[10]

Analytical chemistry:	pP <sub>oct</sub> =	3.44	[21],[24]
	pK <sub>s</sub> =	unknown	
	pK <sub>a</sub> =	4.90	[105]
	pK <sub>BH</sub> =	unknown	
	Henry's law constant =	19.6 kPa·m <sup>3</sup> /mol	[24]
	Hydrolysis half-life =	unknown	

**Electrochemical data:** Meites and Zuman (1977), Meites et al. (1982), Ebersson and Utley (1983b)

**Clay-organic interaction data:** Rao et al. (1988)

**Solubility:** Almost insoluble in water. Very soluble in methanol.

Miscible with ethanol, ether, acetone, benzene, carbon tetrachloride, chlorinated hydrocarbons, and most other organic solvents. [10],[32],[108]

0.01 wt% in water @ 20°C	[10],[49]
<0.01 wt% in water @ 20°C	[32]
57. g/100mL methanol @ 20°C	[108]
57. wt% methanol @ 25°C	[10]

**Form:** Colorless, mobile liquid. Mild, sweet odor resembling benzene, chloroform or gasoline. [107],[32]

**Use:** Solvent to dissolve cellulose ethers, resins, lacquers, fats, waxes, oils, bitumen and crude rubber; paint and varnish remover; in perfume manufacture; during surface coating operations using lacquers; in synthesis of adipic acid and caprolactam for production of Nylon 66 and engineering plastics; in extraction of essential oils; in analytical chemistry for relative molecular mass determinations (cryoscopic constant 20.3); in the manufacture of benzene, cyclohexyl chloride, nitrocyclohexane, cyclohexanol and cyclohexanone; in the manufacture of solid fuel for camp stoves; in fungicidal formulations; and in the industrial recrystallization of steroids. [22],[56],[32]

**Fire and explosion hazard:** Very high.

Flash point: (CC) -20°C [107],[32]

(CC) -17°C [51]

(CC) -18.3°C [49],[22]

UEL: 8.35% [107],[49],[22],[51],[32]

LEL: 1.33% [107],[49],[22],[51],[32]

Autoign. temp.: 245°C [51],[32]

270°C [107]

260°C [49]

500°C [22]

## 232 - Cyclohexane

Extremely flammable liquid. Dangerous fire hazard when exposed to heat or flame. Flashback along vapor trail may occur. Moderate explosion hazard in the form of vapor when exposed to flame. Explodes when mixed hot with liquid  $\text{N}_2\text{O}_4$ . Can react vigorously with oxidizing materials. Fire may release toxic gases and vapors (such as carbon monoxide). Fight fire with foam,  $\text{CO}_2$  or dry chemical. Water may be ineffective as it floats on water. [107],[51]

**Incompatibility:** Strong oxidizing agents;  $\text{N}_2\text{O}_4$ . Will attack some forms of rubber, plastics, and coatings. [56],[51]

**Handling:** Keep away from heat, sparks and flame. Avoid breathing vapor, dust, or mist (appropriate respirator or self-contained breathing apparatus). Avoid contact with eyes, skin and clothing (polyethylene, PVC coated nylon, nitrile or neoprene gloves, apron, and lab coat; chemical safety goggles or face shield). Use with adequate ventilation (fume hood). Keep container tightly closed. Bond and ground container when transferring liquid. Store in cool, dry, well-ventilated flammable liquid storage area. [107],[56],[32]

**Health effects:** Cyclohexane is moderately toxic. It is a local irritant and central nervous system depressant. Routes of entry are inhalation, ingestion, and skin and eye contact. Points of attack include eye, respiratory system, central nervous system, and skin. Short-term exposure may cause dizziness, headache and nausea. Higher levels of exposure may cause unconsciousness. Prolonged or repeated exposure can cause dermatitis due to its defatting action. High concentrations may act as a narcotic. [107],[56],[32]

**Toxicity:** Moderate.

TWA: 300 ppm (1030  $\text{mg}/\text{m}^3$ ) [1]

STEL: no value set [1]

CL: unknown

IDLH: 10000 ppm (34,400  $\text{mg}/\text{m}^3$ ) [107],[56]

Peak: unknown

Odor threshold: 0.41-300 ppm (1.4-1030  $\text{mg}/\text{m}^3$ ) [32]

Carcinogenicity: unknown

Mutagenicity: unknown

**Exposure:**

External:

Non-lethal: 5 ppm (17  $\text{mg}/\text{m}^3$ ) -- eye irritation [32]

>300 ppm (1030  $\text{mg}/\text{m}^3$ ) -- eye and upper respiratory  
irritation [32]

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: 300 ppm (1030  $\text{mg}/\text{m}^3$ ) for 60 min [107]

Non-lethal: >12000 ppm (41,300  $\text{mg}/\text{m}^3$ ) -- depressant effect [32]

Lethal: unknown



DDT

 $C_{14}H_9Cl_5$ 

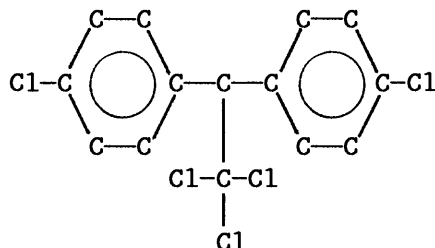
CAS RN: 50-29-3

Syn: DDT \* Benzene, 1,1'-(2,2,2-trichloro-ethylidene)bis[4-chloro- \*  
 Aavero-extra \* Agritan \* Anofex \* Arkotine \* Azotox M-33 \*  $\alpha,\alpha$ -bis(*p*-  
 chlorophenyl)- $\beta,\beta,\beta$ -trichloroethane \* 1,1'-bis(*p*-Chlorophenyl)-2,2,2-  
 trichloroethane \* 2,2-bis(*p*-Chlorophenyl)-1,1,1-trichloroethane \* Bosan  
 supra \* Bovidermol \* Chlorophenotene \* Chlorophenothan \* Chlorophenothane \*  
 Chlorphenothan \* Chlorphenotoxum \* Citox \* Clofenotan \* Clofenotane \* *p,p'*-  
 DDT \* 4,4'-DDT \* Dedelo \* Deoval \* Detox \* Detoxan \* Dibonan \* Dibovin \*  
 Dichlorodiphenyltrichloroethane \* *p,p'*-Dichlorodiphenyltrichloroethane \*  
 4,4'-Dichlorodiphenyltrichloroethane \* Dicophane \* Didigam \* Didimac \*  
 diphenyltrichloroethane \* Dodat \* Dykol \* ENT-1506 \* Estonate \* Genitox \*  
 Gesafid \* Gesapon \* Gesarex \* Gesarol \* Guesapon \* Guesarol \* Gyron \*  
 Havero-extra \* Hildit \* Ivoran \* Ixodex \* Kopsol \* Micro DDT 75 \* Mutoxan \*  
 Mutoxin \* NA-2761 \* NCI-C00464 \* Neocid \* Neocidol (solid) \* OMS-16 \*  
 Parachlorocidum \* PEB<sub>1</sub> \* Pentachlorin \* Pentech \* Penticidum \* Ppzeidan \*  
 R50 \* RCRA Waste Number U061 \* Rukseam \* Santobane \* Tafidex \* Tech DDT \*  
 Trichlorobis(4-chlorophenyl)ethane \* 1,1,1-Trichloro-2,2-bis(*p*-  
 chlorophenyl)ethane \* 1,1,1-Trichloro-2,2-di(4-chlorophenyl)-ethane \*  
 Zeidane \* Zerdane \*

Molecular formula:  $ClC_6H_4C(CCl_3)HC_6H_4Cl$ 

Polychlorinated Hydrocarbon

Structural formula:

**Physical properties:**

Relative molecular mass:	354.49	
Specific gravity:	1.56 @ 15°C	[107]
Boiling point:	260.°C	[105]
	185°C	[8]
Melting point:	109.°C	[10]
	108.5°-109 °C	[105], [108]
	108.°C	[104]
Refractive index:	unknown	
Vapor pressure:	>0. kPa	[104], [108]
	2.0x10 <sup>-8</sup> @ 20°C (1.5x10 <sup>-7</sup> mm)	[8]
	2.5x10 <sup>-8</sup> @ 20°C (1.9x10 <sup>-7</sup> mm)	[41]
	2.2x10 <sup>-11</sup> @ 20°C (1.7x10 <sup>-10</sup> mm)	[41]
	9.7x10 <sup>-8</sup> @ 30°C (7.26x10 <sup>-7</sup> mm)	[41]
	8.3x10 <sup>-11</sup> @ 50°C (6.2x10 <sup>-11</sup> mm)	[41]
Vapor density:	11.5x10 <sup>-9</sup> @ 30°C	[41]
	NA	[107]
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	

## 234 - DDT

Electrical resistivity:	unknown	
Critical temperature:	NA	[107]
Critical pressure:	NA	[107]
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	[107]
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	NA	[107]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	unknown	
Heat of combustion:	NA	[107]
Heat of formation:	unknown	
Gibbs (free) energy:	unknown	

Analytical chemistry:	pP <sub>oct</sub> =	6.19 @ 20°C	[104],[21]
		5.98	[8],[27]
		5.76	[21]
		4.89	[8]
		3.98	[8],[21]
	pK <sub>s</sub> =	NA	
	pK <sub>a</sub> =	NA	[31]
	pK <sub>BH</sub> =	NA	
	Henry's law constant =	0.0104 to 0.00385 kPa-m <sup>3</sup> /mol	[41]
	Hydrolysis half-life =	7.0x10 <sup>6</sup> sec at pH 9	[8]
		3.8x10 <sup>8</sup> sec at pH 3-5	[8]

**Electrochemical data:** Unknown

**Clay-organic interaction data:** Fleck and Haller (1945), Huang and Liao (1970), Karickhoff (1981), Kenega and Goring (1980), McCall et al. (1980), Richardson and Epstein (1971).

**Solubility:** Almost insoluble in water. Slightly soluble in alcohol. Very soluble in ether, acetone, benzene, carbon tetrachloride, kerosine, dioxane, and pyridine. Solubility in organic solvents increases sharply with rise in temperature. [105],[108],[22]

0.0031-0.0034 mg/l water @ 25°C	[104]
58. wt% in acetone	[10]
75. wt% in benzene	[10]
45. wt% in carbon tetrachloride	[10]

**Form:** Colorless crystals or white to slightly off-white powder or waxy solid. Odorless or with slight aromatic odor. DDT is the common name for the technical product of which the predominant component is *p,p'*-DDT with up to 30% of the *o,p'*-isomer. [104],[56],[22]

**Use:** A broad-spectrum non-systemic stomach and contact insecticide; chemical research. Use prohibited in the U.S. [56],[104],[41]

**Fire and explosion hazard:** Moderate

Flash point: 72°-77°C (CC) [107]

uel: NA [107]

lel: NA [107]

Autoign. temp.: unknown

Poisonous gases, such as hydrogen chloride gas, carbon monoxide and carbon dioxide are produced when burned. Fight fire with dry chemical powder, water spray, alcohol or polymer foam. [107],[55]

**Incompatibility:** Strong oxidizers; alkaline materials; bases; iron and iron salts; aluminum. [56],[22],[55]

**Handling:** Self-contained breathing apparatus or appropriate respirator should be worn to prevent inhalation. Use only in well-ventilated area (fume hood). Remove contaminated clothing. Avoid direct eye and skin contact (chemical resistant gloves; safety goggles; other protective clothing). Safety shower and eye bath should be provided. Flush any affected areas including eyes with water. Keep container tightly closed. store in a cool, dry, secure poison area. [107],[55]

**Health effects:** DDT is mildly toxic and an irritant. Routes of entry are inhalation, ingestion, and absorption through skin. Points of attack include central nervous system, blood, liver, kidneys, skin, gastrointestinal system, and peripheral nervous system. Solvents such as kerosene increase toxicity. It is stored in body fat and is a suspected carcinogen. Most concern is for chronic effects. Symptoms are tingling of tongue, lips and face, tremors, apprehension, dizziness, confusion, malaise, headaches, convulsions, paresis of the hands, vomiting, and irritation of eyes and skin. It is irritating to mucous membranes and upper respiratory tract. [108],[56],[107],[51],[55].[69]

**Toxicity:** Moderate

TWA: 0.067 ppm (0.97 mg/m<sup>3</sup>) [56],[1]

STEL: 0.207 ppm (3.0 mg/m<sup>3</sup>) [56]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: NA [107]

Carcinogenicity: suspected [51]

Mutagenicity: suspected [51]

236 - DDT

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: 0.5 mg/kg/day -- no ill effects [104]

250 mg/kg body wt -- acute toxicity [51]

Lethal: 500 mg/kg body wt -- death occurs in 2-24 hrs [108]

221 mg/kg -- death of an adult male [55]

150 mg/kg body wt -- infant death [51]

Inhalation:

Short-term Inhalation Limit: 0.21 ppm (3 mg/m<sup>3</sup>) [107]

Non-lethal: unknown

Lethal: unknown

Dibenz[a,h]anthracene

C<sub>22</sub>H<sub>14</sub>

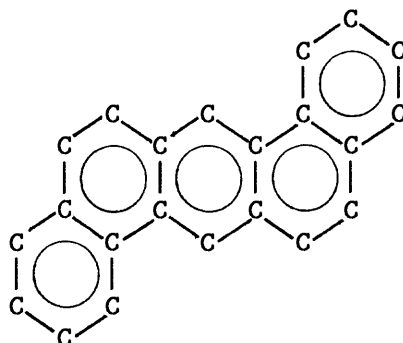
CAS RN: 53-70-3

Syn: Dibenz[a,h]anthracene \* 1,2:5,6-Benzanthracene \* DBA \* DB(a,h)A \*  
 1,2,5,6-DBA \* 1,2:5,6-Dibenzanthracene \* 1,2:5,6-Dibenz(a)anthracene \*  
 Dibenzo(a,h)anthracene \* 1,2:5,6-Dibenzoanthracene \* RCRA Waste Number U063  
 \*

Molecular formula: C<sub>22</sub>H<sub>14</sub>

Polycyclic Aromatic Hydrocarbon

Structural formula:

**Physical properties:**

Relative molecular mass:	278.353	
Specific gravity:	1.282	[41]
	1.252	[59]
Boiling point:	524.°C	[10], [104], [55]
Melting point:	266.°C	[10]
	266.°-267°C	[104]
	269.°-270°C	[105]
Refractive index:	NA	
Vapor pressure:	≈1.3x10 <sup>-11</sup> @ 20°C (1x10 <sup>-10</sup> mm)	[41]
	>0. kPa	[31]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	4.2 μm <sup>2</sup> /s (calc)	[59]
Solution diffusivity:	0.45 nm <sup>2</sup> /s (calc)	[59]
Electric dipole moment:	unknown	
Ionization potential:	7.28 eV	[41]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	31.164 kJ/mol	[105]
Heat of vaporization:	unknown	

## 238 - Dibenz[a,h]anthracene

Heat of sublimation: unknown  
Heat capacity @ 25°C: unknown  
Heat of combustion: unknown  
Heat of formation: unknown  
Gibbs (free) energy: unknown

Analytical chemistry:  $pP_{oct}$  = 6.84 [31]  
6.50 [59]  
6.36 [41]  
5.97 [8]  
 $pK_s$  = NA  
 $pK_a$  = >15. [59]  
NA [31]  
 $pK_{BH}$  = NA  
Henry's law constant =  $7.43 \times 10^{-7}$  kPa-m<sup>3</sup>/mol @20°-25°C(calc) [41]  
 $6.1 \times 10^{-7}$  dimensionless (calc) [59]  
Hydrolysis half-life = NA [8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water, ether. Slightly soluble in acetone and ethanol. Very soluble in benzene, acetic acid, and CS<sub>2</sub>. [10],[105],[41]  
0.0025 mg/L [59]  
0.0005 mg/L @ 25°C [41]  
0.000249 mg/L @ 25°C [41]

Form: Light-yellow crystalline powder; monoclinic or orthorhombic crystals or leaflets. [55],[41]

Use: Not produced commercially; occurs as a contaminant or by-product in wood preservative sludge (0.07 g/L), in high octane gasoline (0.167 mg/L), in coal tar (3.13 mg/g), in cigarette smoke (0.4 $\mu$  g/100 cigarettes), in gasoline engine exhaust, in airborne coal tar emissions, and in coke oven airborne emissions; reserach chemical; derived from industrial and experimental coal gasification operations. [104],[41]

Fire and explosion hazard: Unknown

Flash point: unknown

uel: unknown

lel: unknown

Autoign. temp.: unknown

Decomposition due to heating may produce carbon monoxide and carbon dioxide gas. Fight fire with water spray, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. No other data was found. [55]

Incompatibility: Strong oxidizing agents. [55]

Handling: Avoid all contact. Wear appropriate respirator, chemical resistant gloves, safety goggles, other protective clothing. Wear disposable coveralls and discard them after use. Safety shower and eye bath should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [55]

**Health effects:** DBA is a carcinogen and irritant. Routes of entry are inhalation, ingestion, and skin absorption. The chemical, physical, and toxicological properties have not been thoroughly investigated. [55],[89]

**Toxicity:** Unknown

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: human positive [104]

Mutagenicity: human positive [104]

**Exposure:** Unknown

## 240 - Dibromochloromethane

Dibromochloromethane

CHBr<sub>2</sub>Cl

CAS RN: 124-48-1

Syn: Dibromochloromethane \* Methane, dibromochloro- \* CDBM \*  
 Chlorodibromomethane \* Dibromomonochloromethane \* Monochlorodibromomethane  
 \* NCI-C55254 \*

Molecular formula: CHBr<sub>2</sub>Cl  
 Hydrocarbon

Mixed Halogenated Aliphatic

## Physical properties:

Relative molecular mass:	208.28	
Specific gravity:	2.451	[10],[105]
	2.38	[104],[22]
Boiling point:	118.°-122.°C	[51],[41]
	116.°-122.°C	[104]
Melting point:	<-20.°C	[51],[104]
	-22.°C	[10]
	-23.° - -21.°C	[41]
Refractive index:	1.5482	[105]
	1.5465	[10]
Vapor pressure:	2.0 kPa @ 10.5°C (15mm)	[8],[41]
	10.13 @ 20°C (76mm)	[41]
Vapor density:	7.19	[41]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	unknown	
Kinematic viscosity:	unknown	
Surface tension:	unknown	
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	10.59 eV	[41]
Magnetic volume susceptibility:	-11.10x10 <sup>-6</sup> SI units @ 25°C	[105]
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	unknown	
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	unknown	
Heat of combustion:	unknown	
Heat of formation:	-20.9 kJ/mol @ 25°C (gas)	[10]
Gibbs (free) energy:	-19.84 kJ/mol @ 25°C (gas)	[10]



Analytical chemistry:	$pP_{oct} =$	2.24	[31], [15]
		2.09	[8]
		2.08	[41]
	$pK_s =$	unknown	
	$pK_a =$	12.3 @ 25°C	[52]
	$pK_{BH} =$	unknown	
Henry's law constant =		0.794 kPa·m <sup>3</sup> /mol	[41]
		0.1003	[41]
		0.086 @ 20°C	[24]
Hydrolysis half-life =		8.6x10 <sup>9</sup> sec	[13], [8]

**Electrochemical data:** Unknown

Clay-organic interaction data: Unknown

**Solubility:** Almost insoluble in water. Soluble in ethanol, ether, acetone, benzene, most organic solvents. Miscible with oils, dichloropropane, isopropane. [105],[24]  
0.4 wt% in water @ 22°C [24]

**Form:** Clear, colorless to pale yellow liquid. [51],[104],[56],[22]

Use: Manufacture of fire extinguishing agents, aerosol propellants, refrigerants, pesticides; organic synthesis. [104],[22]

**Fire and explosion hazard:** Very low.

Flash point: none [55]

ue1: NA

1e1: NA

Autoign. temp.: NA

**Non-combustible liquid.** May emit toxic fumes of hydrogen chloride gas, hydrogen bromide gas, CO and CO<sub>2</sub> when heated to decomposition. Use extinguishing media appropriate to surrounding fire conditions. [51],[55]

**Incompatibility:** Strong bases; strong oxidizing agents; magnesium. [55]

**Handling:** Keep away from heat or open flame. Do not breathe vapor or mist (appropriate respirator or self-contained breathing apparatus). Avoid contact with eyes, skin and clothing (chemical resistant gloves; safety goggles; other protective clothing). Use in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Refrigerate. [55]

**Health effects:** Dibromochloromethane is an irritant with narcotic effects. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack are skin, eyes, respiratory system, and central nervous system. It is irritating to skin, eyes, mucous membranes, and upper respiratory tract. Prolonged exposure can cause nausea, dizziness and headache, and narcotic effects. [55]

242 - Dibromochloromethane

Toxicity: Unknown

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: some evidence in mice [26]

Mutagenicity: positive results with *Salmonella typhimurium* TA100 [56]

Exposure: Unknown

1,2-Dibromoethane

 $C_2H_4Br_2$ 

CAS RN: 106-93-4

Syn: 1,2-Dibromoethane \* Ethane, 1,2-dibromo- \* Aadibroom \* Bromofume \* Bromofume 40 \* Celmid \* DBE \* Dibromoethane \* sym-Dibromoethane \*  $\alpha,\beta$ -Dibromoethane \* Dowfume EDB \* Dowfume W-8 \* Dowfume W-85 \* Dowfume W-90 \* Dowfume W-100 \* EDB \* EDB-85 \* E-D-Bee \* ENT 15349 \* Ethylene bromide \* Ethylene dibromide \* 1,2-Ethylene dibromide \* Fumo-gas \* Glycol bromide \* Glycol dibromide \* Iscobrome D \* Kopfume \* NCI-C00522 \* Nefis \* Nephis \* Pestmaster \* Pestmaster EDB-85 \* RCRA Waste Number U067 \* Sanhyuum \* Soilbrom-40 \* Soilbrom-85 \* Soilbrom-90 \* Soilbrom-100 \* Soilbrome-85 \* Soilbrom-90EC \* Soilfume \* UN 1605 (DOT) \* Unifume \*

Molecular formula:  $BrCH_2CH_2Br$ 

Polybrominated Aliphatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	187.86176	
Specific gravity:	2.17-2.18	[22]
	2.1792	[105]
	2.17920	[15]
	2.1791	[49]
	2.1707	[51]
	2.18	[32]
	2.180	[47], [107]
Boiling point:	2.1802	[10]
	131.°C	[32], [22], [56], [107]
	131.36°C	[105]
	131.4°C	[51]
	131.5°C	[47]
	131.6°C	[49], [15], [104]
	131.7°C	[10]
Melting point:	9.10°C	[22]
	9.3°C	[51]
	9.79°C	[105], [49], [15]
	9.8°C	[107]
	9.97°C	[104]
	10.°C	[32], [47], [10]
Refractive index:	1.5416 @ 15°C	[10]
	1.53868	[15]
	1.5387	[105]
	1.53874	[49]
Vapor pressure:	0.133 kPa @ -27.0°C (1mm)	[105], [47]
	0.667 @ 4.7°C (5mm)	[47], [20]
	1.33 @ 18.6°C (10mm)	[105], [47]
	1.467 @ 20°C (11mm)	[32], [104]
	1.04 @ 25°C (7.79mm)	[49]
	1.560 @ 25°C (11.70mm)	[15]
	2.27 @ 30°C (17mm)	[104]
	2.32 @ 30°C (17.4mm)	[51], [22]
	2.67 @ 32.7°C (20mm)	[47], [20]
	5.33 @ 48.0°C (40mm)	[105], [47]
Vapor density:	6.48	[51]
	6.5	[32], [104]
Evaporation rate:	unknown	

## 244 - 1,2-Dibromoethane

Relative dielectric permittivity:	4.912 @ 22.8°C	[2]
	4.991 @ 22.7°C	[2]
	5.010 @ 23.0°C	[2]
	4.63 @ 25°C (1 MHz)	[2]
	4.771 @ 25°C	[15]
	4.78 @ 25°C	[10], [11]
	4.7503 @ 30°C	[49]
	4.1 @ 130°C	[11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	>50. MOhm-m @ 19°C	[49], [10], [11]
Critical temperature:	309.8°C	[49], [10]
Critical pressure:	7.15 MPa	[49], [10]
Dynamic viscosity:	2.438 mPa-s @ 0°C	[105]
	1.880 @ 15°C	[49]
	1.95 @ 17°C	[105]
	1.721 @ 20°C	[105]
	1.490 @ 30°C	[49], [10]
	1.286 @ 40°C	[105]
	0.903 @ 70°C	[105]
	0.750 @ 82.2°C	[105]
	0.648 @ 99°C	[105]
Kinematic viscosity:	1.119 $\mu\text{m}^2/\text{s}$ @ 0°C	
	0.863 @ 15°C	
	0.899 @ 17°C	
	0.790 @ 20°C	
	0.684 @ 30°C	
	0.590 @ 40°C	
	0.414 @ 70°C	
	0.344 @ 82.2°C	
	0.297 @ 99°C	
Surface tension:	38.91 mN/m @ 20°C	[49]
	38.75 @ 20°C	[107]
	38.51 @ 20°C	[15]
	38.37 @ 20°C	[105]
	37.61 @ 30°C	[49]
	37.22 @ 30°C	[15]
	35.13 @ 40°C	[15]
Contact angle:	unknown	
Thermal expansion coefficient:	0.000943 K <sup>-1</sup>	[49]
Compressibility:	0.650 nPa <sup>-1</sup> @ 27°C	[49]
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	3.969x10 <sup>-30</sup> C-m	[49]
	4.10x10 <sup>-30</sup>	[10]
Ionization potential:	10.19 eV (PI)	[105]
Magnetic volume susceptibility:	-11.5x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	10.04 kJ/mol	[15]
	10.84	[105], [107]
	10.945	[49]
	10.97	[10]

Heat of vaporization:	35.87 kJ/mol	[107]
	36.35	[49]
	36.38	[10]
	38.64	[105]
Heat of sublimation:	41.28 kJ/mol	[10]
	58.890	[49]
Heat capacity @ 25°C:	0.1348 kJ/(mol-K) (liq)	[105]
	0.13602 (liq)	[49]
	0.1361 (liq)	[10]
	0.081 (gas)	[105]
Heat of combustion:	-1240.6 kJ/mol @ 25°C (liq)	[49]
Heat of formation:	-81.2 kJ/mol @ 25°C (liq)	[49], [10]
	-38.33 (gas)	[49]
Gibbs (free) energy:	-20.9 kJ/mol @ 25°C (liq)	[10]
Analytical chemistry:	pP <sub>oct</sub> = 1.76	[50]
	pK <sub>s</sub> = unknown	
	pK <sub>a</sub> = unknown	
	pK <sub>BH</sub> = unknown	
	Henry's law constant = unknown	
	Hydrolysis half-life = 5.8x10 <sup>9</sup> sec	[13]

**Electrochemical data:** Meites et al. (1977a).

**Clay-organic interaction data:** Sorption of ethylene dibromide on soil and clay. (Rogers and McFarlane, 1981)

**Solubility:** Slightly soluble in water. Soluble in acetone, benzene.

Miscible with ethanol, ether. Emulsifiable. [105], [47]

0.429 wt% in water @ 30°C	[49]
0.43 wt% in water @ 30°C	[47], [10]
0.431 wt% in water @ 30°C	[104]
0.43 wt% in water @ 25°C	[10]
0.4 wt% in water @ 20°C	[51], [32]

**Form:** Colorless, heavy liquid or solid. Mild, sweet chloroform-like odor. Emulsifiable. [51], [32], [22]

**Use:** In fumigation operations in preplanting and on grains, fruits and vegetables; scavenger for lead in antiknock fluids and fuels; general solvent; in production of water-proofing agents, fire extinguishing agents, and gauge fluids during manufacture of measuring instruments; in organic synthesis in production of dyes, pharmaceuticals and ethylene oxide; as a specialty solvent for resins, gums and waxes. [22], [56]

**Fire and explosion hazard:** Very low

Flash point: NA

l<sub>el</sub>: NA

Autoign. temp.: NA

Nonflammable solid or liquid. Slowly decomposes in the presence of light and heat to form toxic vapors and gases (hydrogen bromide, bromine, carbon monoxide). Reacts with chemically active metals. In case of fire, cool exposed containers with water. Use extinguishing media appropriate to surrounding fire conditions. [51], [32], [55]

## 246 - 1,2-Dibromoethane

**Incompatibility:** Chemically active metals such as sodium, potassium, calcium, powdered aluminum, zinc, magnesium; liquid ammonia; strong oxidizers. [56],[32]

**Handling:** Keep away from light and heat. Avoid breathing vapors (appropriate respirator or self-contained breathing apparatus). Avoid contact with eyes, skin or clothing (rubber gloves, lab coat and apron, chemical safety goggles and face shield). Use with adequate ventilation (fume hood). Safety shower and eye bath stations should be available. Keep container tightly closed. Store in cool, dry, well-ventilated storage area away from heat. **WARNING:** do not use handling equipment or containers composed of magnesium, aluminum or their alloys. [32],[56],[57],[55]

**Health effects:** EDB is a narcotic more poisonous than chloroform, a severe mucous membrane irritant and a hepatic toxin. Routes of entry are inhalation of vapor, ingestion, absorption through skin, and eye or skin contact. Points of attack include respiratory system, liver, kidneys, gastrointestinal system, eyes, and skin. Contact with the skin may cause severe irritation and blistering. Inhalation may cause delayed pulmonary lesions. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. Effects of short-term exposure include irritation to the eyes, nose, throat and skin, and drowsiness. Overexposure or prolonged or repeated exposure may cause damage to the lungs, liver and kidneys, and gastrointestinal disturbances. Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals. Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. [32],[55]

**Toxicity:** Moderate.

TWA: no value set [1]

STEL: no value set [1]

CL: 30 ppm (230 mg/m<sup>3</sup>) [51],[32],[56]

IDLH: 400 ppm (3075 mg/m<sup>3</sup>) [107]

Peak: 50 ppm (385 mg/m<sup>3</sup>) for 5 min duration [51],[32],[56]

Odor threshold: 10-25 ppm (77-192 mg/m<sup>3</sup>) [104]

Carcinogenicity: suspected human carcinogen; results positive for rat and mouse [1],[51],[22],[56],[104],[26]  
a direct-acting carcinogen [103]

Mutagenicity: experimental teratogen, neoplastic effects, equivocal tumorigenic agent [51]  
weakly mutagenic in the *Salmonella* test [104]

**Exposure:**

External:

Non-lethal: 1538 mg for 2 hr -- severe irritation [55]

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: 90 mg/kg body wt -- death of an adult female [51]

Inhalation:

Short-term Inhalation Limits: 50 ppm (385 mg/m<sup>3</sup>) for 5 min [107]

Non-lethal: 25 ppm (190 mg/m<sup>3</sup>) -- tolerable [49]

Lethal: 50 ppm (385 mg/m<sup>3</sup>) -- severe injury and death [49]

Dibutyl phthalate

 $C_{16}H_{22}O_4$ 

CAS RN: 84-74-2

Syn: Dibutyl phthalate \* 1,2-Benzene-dicarboxylic acid, dibutyl ester \* o-Benzenedicarboxylic acid dibutyl ester \* Benzene-o-dicarboxylic acid di-n-butyl ester \* Butyl phthalate \* n-Butyl phthalate \* Celluflex DBP \* DBP \* Dibutyl 1,2-benzenedicarboxylate \* Dibutyl ester phthalic acid \* Di-n-butyl phthalate \* Elaol \* Ergoplast FDB \* Genoplast B \* Hexaplas M/B \* NA 9095 \* Palatinol C \* Phthalic acid, dibutyl ester \* Polycizer DBP \* PX 104 \* RCRA Waste Number U069 \* RC plasticizer DBP \* Staflex DBP \* Unimoll DB \* Witcizer 300 \*

Molecular formula: 1,2- $C_6H_4(COO(CH_2)_3CH_3)_2$ 

Dicarboxylic Acid Ester

**Physical properties:**

Relative molecular mass:	278.348	
Specific gravity:	1.05	[32]
	1.049	[107]
	1.0465	[10], [49], [104]
Boiling point:	340.°C	[105], [104], [22], [10]
	335.°C	[107], [32]
Melting point:	-35.°C	[49], [104], [22]
	-37.°C	[32]
Refractive index:	1.4911 @ 20°C	[105]
	1.4926 @ 20°C	[10], [49]
Vapor pressure:	<0.0013 kPa @ 20°C (0.01mm)	[32]
	0.01 @ 89°C (0.07mm)	[49]
Vapor density:	9.61	[41]
	9.58	[51], [32]
Evaporation rate:	≈0.	[32]
Relative dielectric permittivity:	6.436 @ 30°C	[10], [49], [11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	0.238 MOhm-m @ 30°C	[49]
	5.555 @ 30°C	[11]
Critical temperature:	500.°C	[107]
Critical pressure:	1.7 MPa	[107]
Dynamic viscosity:	20.3 mPa-s @ 20°C	[22]
	15.4 @ 25°C	[49]
	16.47 @ 25°C	[10]
	2.2 @ 100°C	[49]
Kinematic viscosity:	19.39 $\mu m^2/s$ @ 20°C	
	14.7 @ 25°C	
	2.1 @ 100°C	
Surface tension:	33.40 mN/m @ 20°C	[10], [49]
	34. @ 20°C	[107]
Contact angle:	unknown	
Thermal expansion coefficient:	0.00086 K <sup>-1</sup>	[49]
Compressibility:	unknown	
Vapor diffusivity:	4.2 $\mu m^2/s$ @ 25°C	[59]
Solution diffusivity:	0.41 nm <sup>2</sup> /s (calc)	[59]
Electric dipole moment:	8.005x10 <sup>-30</sup> C-m	[10]
	9.41x10 <sup>-30</sup>	[49]
Ionization potential:	unknown	

## 248 - Dibutyl phthalate

Magnetic volume susceptibility:	-8.26x10 <sup>-6</sup> @ 21°C	[105]
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	79.2 kJ/mol	[49]
	74.30	[105]
Heat of sublimation:	91.69 kJ/mol	[10]
Heat capacity @ 21°C:	0.498 kJ/(mol-K)	[49]
Heat of combustion:	-8611. kJ/mol (liq)	[49]
	-8624. (liq)	[107]
Heat of formation:	-841.5 kJ/mol @ 25°C (sol)	[10]
	1025. (liq)	[49]
Gibbs (free) energy	-523.4 kJ/mol (gas) (calc)	[59]
Analytical chemistry: pP <sub>oct</sub> =		
	5.56	[31]
	5.2	[8]
	4.72	[23]
	4.31	[41]
	pK <sub>s</sub> =	NA
	pK <sub>a</sub> =	NA
	pK <sub>BH</sub> =	NA
Henry's law constant =	0.00064 kPa-m <sup>3</sup> /mol	[41]
	0.000074 dimensionless	[59]
Hydrolysis half-life =	3.15x10 <sup>8</sup> sec	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Very slightly soluble in water. Very soluble in ethanol, ether, acetone, benzene. [10],[32],[104]

0.45 wt% in water @ 20°C	[32]
0.003 wt% in water @ 20°C	[59]
0.04 vol% in water @ 25°C	[104]
0.01 wt% in water @ 25°C	[10],[23]

Form: Colorless, oily liquid. Very weak, aromatic odor. [32]

Use: Liberated during spraying application of polyvinyl acetate surface coatings, during spray application of polyester and epoxy resins, during hand and dip applications of polyvinyl acetate, and polyester and epoxy resins, during molding and forming of cellulose acetate butyrate, acetate, propionate, and polyvinyl acetate, during application of polyvinyl acetate adhesives, during manufacture of nitrile rubber, during molding of polyester and epoxy articles; in spray application of nitrocellulose lacquer surface coatings; insect repellent; as plasticizer in elastomers; explosives; nail polish; solid rocket propellants; solvent for perfume oils; perfume fixative; textile lubricating agent; in safety glass, printing inks, resin solvents, paper coatings, adhesives. [22],[56],[32]



**Fire and explosion hazard:** Low.

Flash point: (CC) 157°C [107],[51],[32]

(OC) 179°C [107]

(OC) 171°C [49],[22]

uel: 2.5% [107]

lel: 0.5% [107]

0.47% @ 236°C [55]

Autoign. temp.: 403°C [107],[49],[51],[32]

Slightly flammable liquid. Slight fire hazard when exposed to heat, flame, or incompatible substances. Violent reaction with chlorine. Fire may emit toxic gases and vapors (such as CO and CO<sub>2</sub>). Fight fire with CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. Water or foam may cause frothing. [51],[32]

**Incompatibility:** Nitrates; strong oxidizers; strong bases; strong acids; chlorine. [56],[51],[32]

**Handling:** Avoid heat, flame and other sources of ignition. Avoid eye and skin contact (nitrile, PVA synthetic latex or neoprene gloves and lab coat; chemical goggles or face shield). Do not breath vapor or mist (appropriate respirator or self-contained breathing apparatus). Use in well-ventilated area (fume hood). Safety shower and eye bath should be available. Keep container tightly closed. Store in cool, dry, well-ventilated area. [107],[55]

**Health effects:** Di-n-butyl phthalate is relatively non-toxic. Routes of entry are inhalation, ingestion, skin absorption, and skin and eye contact. Points of attack include respiratory system, central nervous system, skin, and eyes. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Swallowing may cause nausea, dizziness, light sensitivity, watering and redness of the eyes, and irritation of nasal passages and upper respiratory system. Overexposure to hot vapors or mists may produce nausea, dizziness, headache, drowsiness and convulsions. At industrial exposure levels, it is relatively nonirritating to the skin, eyes, and mucous membranes. DBP is practically harmless to the skin. Vapors may or may not be toxic. [107],[56],[32],[49],[55]

**Toxicity:** Low.TWA: 0.5 ppm (5 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: 817 ppm (9300 mg/m<sup>3</sup>) [107],[56]

Odor threshold: unknown

Carcinogenicity: unknown

Mutagenicity: positive laboratory experiments [55]

**Exposure:**

External: unknown

Oral:

Non-lethal: 140 mg/kg body wt -- systemic eye effects [51]

Lethal: unknown

Inhalation: unknown

## 250 - 1,2-Dichlorobenzene

1,2-Dichlorobenzene

 $C_6H_4Cl_2$ 

CAS RN: 95-50-1

Syn: 1,2-Dichlorobenzene \* Benzene, 1,2-dichloro- \* Chloroben \* Chloroden  
 \* DCB \* o-DCB \* 1,2-DCB \* o-Dichlorbenzene \* o-Dichlor benzol \* *ortho*-  
 Dichlorobenzene \* Dichlorobenzene \* o-Dichlorobenzene \* Dichlorobenzene,  
*ortho*, liquid \* o-Dichlorobenzol \* Dilantin DB \* Dilatin DB \* Dizene \*  
 Dowtherm E \* NCI-C54944 \* ODB \* ODCB \* Orthodichlorobenzene \*  
 Orthodichlorobenzol \* RCRA Waste Number U070 \* Special termite fluid \*  
 Termitkil \* UN 1591 (DOT) \*

Molecular formula:  $C_6H_4Cl_2$ 

Polychlorinated Aromatic Hydrocarbon

## Physical properties:

Relative molecular mass:	147.004		
Specific gravity:	1.306		[107], [108]
	1.3059		[10]
	1.305		[104], [47]
	1.3048		[105]
Boiling point:	180.°-183°C		[51]
	180.5°C		[105], [107], [108]
	180.48°C		[49]
	180.4°C		[10]
	179.°C		[104], [56], [47]
	172.°-179°C		[22]
Melting point:	-16.7°C		[104]
	-17.°C		[105]
	-17.01°C		[49]
	-17.2°C		[10]
	-17.5°C		[51]
	-17.6°C		[107], [47], [32]
	-18.°C		[104]
	-22.°C		[51]
Refractive index:	1.55145		[49]
	1.5505		[10], [105]
Vapor pressure:	0.133 kPa @ 20°C	(1mm)	
	[104], [105], [47]		
	0.171	@ 25°C	(1.28mm) [49]
	0.200	@ 25°C	(1.5mm) [104]
	0.253	@ 30°C	(1.9mm) [104]
	1.333	@ 59.1°C	(10mm) [105]
	5.333	@ 89.4°C	(40mm) [105]
	5.1		[32]
Vapor density:	5.07		[104]
	5.05		[51]
	0.15		[49]
Evaporation rate:	0.15		[49]
Relative dielectric permittivity:	9.93 @ 25°C		[49], [10], [105], [20]
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	unknown		
Electrical resistivity:	333. MOhm-m @ 25°C		[49]
Critical temperature:	424.1°C		[49]
Critical pressure:	4.10 MPa		[49]
Dynamic viscosity:	1.324 mPa-s @ 25°C		[10]
Kinematic viscosity:	1.013 $\mu m^2/s$ @ 25°C		

Surface tension:	37. mN/m @ 20°C	[107]	
	26.84 @ 20°C	[49]	
	35.55 @ 30°C	[49]	
Contact angle: [18]			
	sessile	advancing	receding
quartz	24	24	16
calcite	30	32	11
biotite	22	22	11
Ca-mont.	6	6	0
Thermal expansion coefficient:	0.00085 K <sup>-1</sup>	[49]	
Compressibility:	unknown		
Vapor diffusivity:	unknown		
Solution diffusivity:	unknown		
Electric dipole moment:	8.339x10 <sup>-30</sup> C-m	[105], [10]	
Ionization potential:	9.06 eV (PI)	[105]	
Magnetic volume susceptibility:	-9.40x10 <sup>-6</sup> SI units @ 20°C	[105]	
Speed of sound:	unknown		
Heat of melting:	13.36 kJ/mol	[10]	
	12.929	[105]	
	12.94	[107], [47]	
	12.59	[49]	
Heat of vaporization:	45.816 kJ/mol	[105]	
	40.61	[10]	
	39.40	[107]	
	39.66 @ bp	[49]	
	50.21 @ 25°C	[49]	
Heat of sublimation:	48.40 kJ/mol	[10]	
Heat capacity @ 25°C:	0.1135 kJ/(mol-K) (gas)	[10]	
	0.22167 (liq)	[49]	
Heat of combustion:	-2958.63 kJ/mol @ 25°C (liq)	[49]	
	-2812.69 (liq)	[105]	
	-2724.82 (liq)	[107]	
Heat of formation:	-18.07 kJ/mol @ 25°C (liq)	[49]	
	29.98 (gas)	[10]	
	29.7 (gas)	[49]	
Gibbs (free) energy:	82.73 kJ/mol (gas)	[10]	
Analytical chemistry: pP <sub>oct</sub> =	3.56	[31]	
	3.55	[41]	
	3.40	[4]	
	3.39	[27]	
	3.38	[104], [23], [8], [12]	
	pK <sub>s</sub> = unknown		
	pK <sub>a</sub> = 2.92	[105]	
	pK <sub>BH</sub> = unknown		
Henry's law constant =	0.12 kPa-m <sup>3</sup> /mol @ 20°C	[41]	
	0.24 @ 25°C	[41]	
	0.287 @ 37°C	[41]	
Hydrolysis half-life =	NA	[8]	

Electrochemical data: Unknown

Clay-organic interaction data: Chiou et al. (1983)

## 252 - 1,2-Dichlorobenzene

**Solubility:** Insoluble in water. Soluble in ethanol, ether, acetone, benzene, carbon tetrachloride. [104],[49],[105],[47],[32]

0.0100 wt% in water @ 20°C	[10],[104]
0.0145 wt% in water @ 25°C	[104]
0.0156 wt% in water @ 25°C	[23],[49]
0.015 wt% in water @ 20°C	[32]

**Form:** Clear to pale-yellow liquid. Characteristic, aromatic, pleasant odor. Technical grades are as follows -- Pure: not less than 99.5% *ortho*, not more than 0.5% *para*; Technical grades: up to 17% *para* and 2% *meta* isomers. [56],[107]

**Use:** Process solvent in the manufacturing of toluene diisocyanate, 3,4-dichloro-aniline; intermediate in the synthesis of dyestuffs, fumigants, herbicides, and degreasers; industrial air/odor control; metal polishes; solvent for a wide variety of organic compounds and for nonferrous metal oxides; heat transfer medium. [22],[56],[108],[32],[41]

**Fire and explosion hazard:** Moderate

Flash point: (CC) 68.33°C [107]  
(CC) 66.1°C [51],[49],[108]  
(OC) 73.89°C [107]

UEL: 9.2% [51],[107]

LEL: 2.2% [51],[107]

Autoign. temp.: 647.8°C [51],[22],[107]

Flammable liquid. Combustion releases irritating vapors such as hydrogen chloride gas, chlorocarbons, chlorine, CO and CO<sub>2</sub>. Fight fire with water, alcohol or polymer foam, dry chemical powder, CO<sub>2</sub>. [107]

**Incompatibility:** Strong oxidizers; hot aluminum or aluminum alloys; sensitive to light. [56],[55]

**Handling:** Keep away from heat and open flame. Do not breathe vapor (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, on clothing (butyl rubber or chlorinated polyethylene gloves and overclothing; safety goggles or face shield). Readily absorbed through skin. Prevent repeated or prolonged skin contact. Remove nonimpervious clothing if wet or contaminated and wash promptly if skin is wet or contaminated. Safety shower and eye bath should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet away from light. [56],[32],[107],[53],[55]

**Health effects:** o-DCB is moderately toxic. Routes of entry are inhalation, ingestion, skin absorption, and skin and eyes. Points of attack include lungs, central nervous system, liver, kidneys, skin, and eyes. It is irritating to mucous membranes and upper respiratory tract. May cause allergic skin reaction. Exposure can cause hemolytic anemia and liver necrosis. High concentrations cause central nervous system depression. Chronic overexposure may cause liver and kidney damage and possible carcinogenic effects. [22],[56],[108],[55]

**Toxicity: Moderate**

TWA: no value set [1]

STEL: no value set [1]

CL: 50 ppm (300 mg/m<sup>3</sup>) [1],[56],[51]IDLH: 1700 ppm (10,200 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 4-50 ppm (24-300 mg/m<sup>3</sup>) [107]

Carcinogenicity: inadequate human evidence [55]

inadequate animal evidence [55]

negative response in small animals [26]

Mutagenicity: unknown

**Exposure:**

## External:

Non-lethal: 20-30 ppm (120-180 mg/m<sup>3</sup>) -- eye irritation [32]

Lethal: unknown

## Oral:

Non-lethal: unknown

Lethal: unknown

## Inhalation:

Short-term Inhalation Limits: <300 ppm (<1800 mg/m<sup>3</sup>) for 60 min [104]Non-lethal: 1-44 ppm (6-265 mg/m<sup>3</sup>) -- no injuries [104]>25 ppm (>150 mg/m<sup>3</sup>) -- unsatisfactory [104]100 ppm (600 mg/m<sup>3</sup>) -- irritating odors [104]100 ppm (600 mg/m<sup>3</sup>) -- symptoms of illness appear [104]

Lethal: unknown

## 254 - 1,3--Dichlorobenzene

1,3-Dichlorobenzene

 $C_6H_4Cl_2$ 

CAS RN: 541-73-1

Syn: 1,3-Dichlorobenzene \* Benzene, 1,3-dichloro- \* *m*-Dichlorobenzene \* *m*-Dichlorobenzol \* Metadichlorobenzene \* *m*-Phenylene dichloride \* RCRA Waste Number U071 \* UN 1591 (DOT) \*

Molecular formula:  $C_6H_4Cl_2$ 

Polychlorinated Aromatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	147.004		
Specific gravity:	1.28844°C	[10], [105], [49], [107]	
	1.288°C	[104], [22], [47]	
Boiling point:	173.1°C	[10]	
	173.°C	[49], [105], [107]	
	172.°C	[104], [22], [47], [10]	
Melting point:	-24.8°C	[10]	
	-24.76°C	[49], [104], [105], [47], [107]	
	-24.°C	[22]	
Refractive index:	1.54586	[49], [105]	
	1.5459	[10]	
Vapor pressure:	0.133 kPa @ 12.1°C (1mm)	[105]	
	0.252 @ 25°C (1.89mm)	[49]	
	0.307 @ 25°C (2.3mm)	[23]	
	0.666 @ 38.8°C (5mm)	[55]	
	1.33 @ 52°C (10mm)	[105], [47]	
	5.333 @ 82.0°C (40mm)	[105]	
Vapor density:	5.07	[107]	
Evaporation rate:	unknown		
Relative dielectric permittivity:	5.04 @ 25°C	[10], [49], [105], [11]	
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	unknown		
Electrical resistivity:	unknown		
Critical temperature:	410.8 °C	[49], [107]	
Critical pressure:	3.8 MPa	[49], [107]	
Dynamic viscosity:	1.04 mPa-s @ 25°C	[10]	
Kinematic viscosity:	0.8112 $\mu m^2/s$ @ 25°C		
Surface tension:	33.16 mN/m @ 20°C	[49]	
	36.01 @ 20°C	[107]	
	33.53 @ 41.8°C	[49]	
Contact angle:	unknown		
Thermal expansion coefficient:	unknown		
Compressibility:	unknown		
Vapor diffusivity:	unknown		
Solution diffusivity:	unknown		
Electric dipole moment:	5.137x10 <sup>-30</sup> C-m @ 25°C	[49]	
	5.737x10 <sup>-30</sup> @ 25°C	[105], [10]	
Ionization potential:	9.12 eV (PI)	[105]	
Magnetic volume susceptibility:	-9.16x10 <sup>-6</sup> SI units @ 20°C	[105]	
Speed of sound:	unknown		
Heat of melting:	12.65 kJ/mol	[107]	
	12.64	[105]	

Heat of vaporization:	48.58 kJ/mol @ 25°C	[49]
	38.63 @ 173°C	[49], [107]
	43.74	[105]
Heat of sublimation:	47.90 kJ/mol @ 25°C	[10]
Heat capacity @ 25°C:	0.11385 kJ/(mol-K) (gas)	[49]
@ 25°C:	0.1139 (gas)	[10]
@ 0°C:	0.1656 (liq)	[47]
Heat of combustion:	-2955.75 kJ/mol @ 25°C (liq)	[49]
	-2914.43 @ 25°C (liq)	[20]
	-2768.41 @ 25°C (liq)	[107]
Heat of formation:	-20.92 kJ/mol @ 25°C (liq)	[49]
	-20.10 @ 25°C (liq)	[20]
	25.5 @ 25°C (gas)	[49]
	26.46 @ 25°C (gas)	[10]
Gibbs (free) energy:	78.63 kJ/mol @ 25°C (gas)	[10]
Analytical chemistry: p <sub>Oct</sub> =	3.60	[23]
	3.56	[31]
	3.48	[12], [27]
	3.44	[4]
	3.38	[104], [8], [21]
	pK <sub>s</sub> = unknown	
	pK <sub>a</sub> = 3.82	[105]
	pK <sub>BH</sub> = unknown	
Henry's law constant =	0.365 kPa-m <sup>3</sup> /mol	[41]
	0.266	[41]
	0.476 @ 25°C	[41]
	0.469 @ 37°C	[41]
Hydrolysis half-life =	NA	[8]
Electrochemical data: Unknown		
Clay-organic interaction data: Chiou et al. (1983)		
Solubility: Almost insoluble in water. Soluble in ethanol, ether, acetone, benzene, carbon tetrachloride. [49],[104],[105],[47]		
	0.0111 wt% in water @ 20°C	[10], [49]
	0.0069 wt% in water @ 22°C	[104]
	0.0123 wt% in water @ 25°C	[104]
Form: Colorless liquid. [22],[107]		
Use: Usually occurs as a contaminant of 1,2-dichlorobenzene and 1,4-dichlorobenzene production. Uses include: fumigant and insecticide; organic synthesis. [22],[41]		

## 256 - 1,3--Dichlorobenzene

### Fire and explosion hazard: Low

Flash point: (CC) 151°C (est) [107]  
(OC) 165°C (est) [107]  
(??) 63°C [41]

uel: 9.2% (est) [107]

lel: 2.02% (est) [107]

Autoign. temp.: 648°C (est) [107]

Flammable liquid. Irritating vapors including hydrogen chloride are produced when burned. Fight fire with CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [107],[55]

**Incompatibility:** Oxidizing agents; aluminum and its alloys. [55]

**Handling:** Keep away from heat and open flame. Do not breathe vapor (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (butyl rubber or chlorinated polyethylene gloves and suit; safety goggles or face shield). Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [107],[53],[55]

**Health effects:** 1,3-DCB is an irritant. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include liver, kidney, upper respiratory tract, gastrointestinal tract, skin, and eyes. It is irritating to eyes, skin, mucous membranes, and upper respiratory tract. Inhalation may cause headache, drowsiness, unsteadiness, and irritating to mucus membranes, eyes, and skin. Ingestion may cause nausea, vomiting, diarrhea, abdominal cramps and cyanosis. Overexposure may cause liver and kidney damage. [107],[55]

### Toxicity: Moderate

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: 0.02 ppm (0.12 mg/m<sup>3</sup>) in water [107]

Carcinogenicity: unknown

Mutagenicity: unknown

**Exposure:** Unknown



1,4-Dichlorobenzene

 $C_6H_4Cl_2$ 

CAS RN: 106-46-7

Syn: 1,4-Dichlorobenzene \* Benzene, 1,4-dichloro- \* p-Chlorophenyl chloride \* Di-chloricide \* 1,4-DCB \* p-Dichlorobenzene \* Dichlorobenzene, para, solid \* p-Dichlorobenzol \* Dichlorocide \* Evola \* Globol \* NCI-C54955 \* Paracide \* Para Crystals \* Paradi \* Paradichlorobenzene \* Paradichlorobenzol \* Paradow \* Paramoth \* Paranuggets \* Parazene \* Parodi \* PDB \* PDCB \* Persia-perazol \* RCRA Waste Number U072 \* Santochlor \* UN 1592 (DOT)

Molecular formula: 1,4- $C_6H_4Cl_2$ 

Polychlorinated Aromatic Hydrocarbon

## Physical properties:

Relative molecular mass:	147.004	
Specific gravity:	1.458	[22], [56], [107]
	1.46	[32]
	1.2475	[105]
Boiling point:	174.55°C	[106]
	174.2°C	[107]
	174.12°C	[49]
	174.1°C	[10]
	174.°C	[47], [32], [56], [105]
	173.7°C	[22]
	173.4°C	[104], [51]
Melting point:	53.13°C (sublimes readily)	[49]
	53.1°C	[106], [105]
	53.°C	[10], [47], [32], [22], [104], [107]
Refractive index:	1.5285 @ 20°C	[106], [105]
	1.5285 @ 60°C	[10]
	1.52849 @ 60°C	[49]
Vapor pressure:	0.053 kPa @ 20°C	(0.4mm) [32]
	0.080 @ 20°C	(0.6mm) [56]
	0.235 @ 25°C	(1.76mm) [49], [23]
	0.240 @ 30°C	(1.8mm) [56]
	1.333 @ 54.8°C	(10mm) [105], [51]
	5.333 @ 84.8°C	(40mm) [105]
Vapor density:	5.08	[51]
	5.07	[56], [104]
	5.1 @ bp	[32]
Evaporation rate:	NA	[32]
Relative dielectric permittivity:	2.41 @ 50°C	[49], [10], [105]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	411.6°C	[14]
Critical pressure:	3.91 MPa	[14]
Dynamic viscosity:	0.720 mPa-s @ 70°C	[10]
Kinematic viscosity:	0.494 $\mu m^2/s$ @ 70°C	

## 258 - 1,4-Dichlorobenzene

Surface tension:	34.66 mN/m @	0°C	[10]
([10] values calculated)	33.78	@ 10°C	[10]
	32.90	@ 20°C	[10]
	32.02	@ 30°C	[10]
	31.14	@ 40°C	[10]
	30.26	@ 50°C	[10]
	29.39	@ 60°C	[10]
	30.69	@ 68°C	[49]
	28.51	@ 70°C	[10]
	27.58	@ 96°C	[49]
	25.87	@ 100°C	[10]

Contact angle: [18]

	sessile	advancing	receding
quartz	23	22	14
calcite	26	25	13
biotite	22	24	13
Ca-mont.	5	8	5

Thermal expansion coefficient: unknown

Compressibility: unknown

Vapor diffusivity: unknown

Solution diffusivity: unknown

Electric dipole moment: 0. [49], [10], [105]

Ionization potential: 8.95 eV (PI) [105]

Magnetic volume susceptibility:  $-10.34 \times 10^{-6}$  SI units @ 20.5°C [105]

Speed of sound: unknown

Heat of melting: 18.187 kJ/mol [49]

18.17 [10]

17.89 [107]

17.15 [105]

Heat of vaporization: 72.266 kJ/mol [105]

49.0 @ 25°C [49]

44.426 [105]

39.77 [10]

38.79 @ bp [49]

Heat of sublimation: 64.90 kJ/mol [10]

64.77 [49]

Heat capacity @ 25°C: 0.167 kJ/(mol-K) (sol) [49]

@ 57°C: 0.1842 (liq) [49]

@ 25°C: 0.1140 (gas) [10]

Heat of combustion: -2934.11 kJ/mol @ 25°C (sol) [49]

-2888.9 (liq) [20]

Heat of formation: -42.3 kJ/mol @ 25°C (liq) [20]

23.03 (gas) [10]

Gibbs (free) energy: 77.20 @ 25°C (gas) [10]

Analytical chemistry:  $pP_{oct}$  = 3.56 [31]

3.52 [23]

3.39 @ 20°C [56], [8], [21]

3.38 [12], [27]

3.37 [4]

$pK_s$  = unknown

$pK_a$  = 3.98 @ 25°C [105]

$pK_{BH}$  = unknown

Henry's law constant =	0.456 kPa-m <sup>3</sup> /mol @ 25°C	[41]
	0.31	[41]
	0.276	[41]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Meites and Zuman (1977), Meites et al. (1982)

Clay-organic interaction data: Chiou et al. (1983)

Solubility: Almost insoluble in water. Slightly soluble in ether, benzene, chloroform, carbon disulfide. Miscible in ethanol, acetone. [105],[47],[56],[104],[49],[32]

0.008	wt% in water @ 20°C	[32]
0.0049	wt% in water @ 22°C	[56],[104]
0.0079	wt% in water @ 25°C	[56],[104]
0.00872	wt% in water @ 25°C	[49]
0.01	wt% in water @ 35°C	[10]
0.021	wt% in water @ 59.2°C	[49]

Form: Colorless or white crystals. Penetrating, aromatic, mothball-like odor. [32],[56]

Use: Ninety percent of total production is for use in production of insecticides or air deodorants. It is also used in the manufacture of dyes and intermediates, pharmaceuticals, moth repellants; soil fumigant; pesticide. [56],[32]

Fire and explosion hazard: Low

Flash point: (CC) 65.5°C [51],[107],[22]  
(OC) 73.9°C [107]  
(OC) 67°C [49]

uel: unknown

lel: 2.5% (calculated at flash point) [32]

Autoign. temp.: unknown

Low flammability solid. Can react vigorously with oxidizing materials. Toxic gases and vapors (such as hydrogen chloride gas, CO and CO<sub>2</sub>) may be released when heated to decomposition. Cool exposed containers with water. Fight fire with water, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [32],[55]

Incompatibility: Oxidizing agents; aluminum and its alloys. [55]

Handling: Avoid heat, open flame, and sources of ignition. Prevent inhalation of dust or fumes (appropriate respirator). Do not get in eyes, on skin, on clothing (chemical resistant gloves, safety goggles, other protective clothing). Remove nonimpervious clothing promptly if wet or contaminated. Use with adequate ventilation (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry place. [56],[107],[55]

## 260 - 1,4-Dichlorobenzene

**Health effects:** 1,4-DCB is moderately toxic. Routes of entry are: inhalation, ingestion, and skin and eye contact. Points of attack include: respiratory tract, gastrointestinal system, liver, kidneys, skin, and eyes. It is irritating to mucous membranes and upper respiratory tract. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. It may cause allergic skin reaction. Chronic overexposure can cause damage to the liver and kidneys and may cause carcinogenic effects. Other symptoms include: headaches, eye irritation, periorbital swelling, profuse rhinitis, anorexia, nausea, vomiting, weight loss, jaundice, and cirrhosis. [32],[56],[55]

**Toxicity:** Moderate to high

TWA: 75 ppm (450 mg/m<sup>3</sup>) [56],[51],[1]

STEL: 110 ppm (660 mg/m<sup>3</sup>) [56],[1]

CL: unknown

IDLH: 1000 ppm (6000 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 15-30 ppm (90-180 mg/m<sup>3</sup>) [32],[107],[56]

Carcinogenicity: suspected [51]

inadequate evidence [55]

positive response in mice [26]

Mutagenicity: suspected [51]

**Exposure:**

**External:**

Non-lethal: 50-80 ppm (300-480 mg/m<sup>3</sup>) -- painful to eyes and nose [32]

160 ppm (960 mg/m<sup>3</sup>) -- severe discomfort [32]

Lethal: unknown

**Oral:**

Non-lethal: 300 mg/kg body wt -- systemic effects [51]

Lethal: 221 mg/kg body wt -- death of an adult male [51]

857 mg/kg [55]

357 mg/kg [55]

**Inhalation:**

Non-lethal: 15-85 ppm (90-500 mg/m<sup>3</sup>) -- no injuries [32]

160 ppm (960 mg/m<sup>3</sup>) -- severe discomfort [32]

Lethal: unknown

Dichlorodifluoromethane

CCl<sub>2</sub>F<sub>2</sub>

CAS RN: 75-71-8

Syn: Dichlorodifluoromethane \* Methane, dichlorodifluoro- \* Algofrene type 2 \* Arcton 6 \* Arcton 12 \* Difluorodichloromethane \* Electro-CF 12 \* Eskimon 12 \* F-12 \* FC 12 \* Fluorocarbon-12 \* Freon 12 \* Frigen 12 \* Genetron 12 \* Halon \* Halon 122 \* Isceon 122 \* Isotron 12 \* Kaiser Chemicals 12 \* Ledon 12 \* Propellant 12 \* R 12 \* R 12 (refrigerant) \* RCRA Waste Number U075 \* Refrigerant 12 \* Ucon 12 \* Ucon 12/halocarbon 12 \* UN 1028 (DOT) \*

Molecular formula: CCl<sub>2</sub>F<sub>2</sub>

Mixed Halogenated Aliphatic Halide

**Physical properties:**

Relative molecular mass:	120.914		
Specific gravity:	1.3292 @ 20°C (liq)		[104], [49]
	1.311 @ 25°C (liq)		[105]
Boiling point:	-29.°C		[51]
	-29.77°C		[49]
	-29.8°C	[10], [105], [107], [104], [22]	
	-30.°C		[56]
Melting point:	-111.°C		[104]
	-157.7°C		[107]
	-158.°C	[10], [105], [51], [104], [22]	
	-158.2°C		[49]
Refractive index:	1.2950		[49]
Vapor pressure:	202.65 @ -12.2°C (1520mm)	[105], [20]	
	506.62 @ 16.1°C (3800mm)	[51], [20]	
	566.62 @ 20°C (4250mm)	[49], [104]	
	770.07 @ 30°C (5776mm)	[104]	
	1013.25 @ 42.4°C (7600mm)	[105], [20]	
Vapor density:	4.2	[107], [32]	
	4.18	[104]	
	4.17	[105]	
Evaporation rate:	380.	[32]	
Relative dielectric permittivity:	2.13 @ 29°C (liq)	[49], [105]	
	1.0016 @ 29°C (380mm) (gas)	[105]	
	1.00029 @ 0°-100°C (760mm) (gas)	[105]	
Loss tangent:	NA		
Relaxation time:	NA		
Thermal conductivity:	0.09169 W/(m-K) @ -17.8°C	[105]	
	0.09865 @ -6.67°C	[47]	
	0.09173 @ 15.56°C	[47]	
	0.07096 @ 25°C (liq)	[105]	
	0.07117 @ 25°C	[49]	
	0.08307 @ 37.78°C	[47]	
	0.07442 @ 60°C	[47]	
	0.09671 @ 0-75°C	[105]	
	0.00968 @ 25°C (gas)	[105]	
Electrical resistivity:	NA		
Critical temperature:	111.8°C	[49], [107], [10]	
	111.5°C	[105], [47]	
	112.°C	[105]	

## 262 - Dichlorodifluoromethane

Critical pressure:	4.38 MPa	[22]
	4.125	[49], [10]
	4.12	[107]
	4.11	[105]
	4.013	[105]
	4.008	[47]
Dynamic viscosity:	0.32 mPa-s @ -15°C	[49]
	0.26 @ 25°C (liq)	[105]
	0.22 @ 30°C	[49]
	0.013 @ 25°C (gas)	[105]
Kinematic viscosity:	0.241 $\mu\text{m}^2/\text{s}$ @ -15°C	
	0.196 @ 25°C (liq)	
	0.166 @ 30°C	
	0.010 @ 25°C (gas)	
Surface tension:	9. mN/m @ 25°C	[49], [105]
Contact angle:	NA	
Thermal expansion coefficient:	NA	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	1.7x10 <sup>-30</sup> C-m	[105]
	1.83x10 <sup>-30</sup>	[49]
Ionization potential:	12.31 eV (PI)	[105]
Magnetic volume susceptibility:	-8.07x10 <sup>-6</sup> SI units @-30°C	[105]
Speed of sound:	unknown	
Heat of melting:	4.14 kJ/mol	[49]
Heat of vaporization:	39.417 kJ/mol	[107]
	35.0146	[105]
	20.112 @ bp	[49]
	19.98 @ bp	[105]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.1172 kJ/(mol-K) (???)	[49]
	0.0723 (gas)	[105]
	0.0610 (gas)	[10]
Heat of combustion:	-1481.6 kJ/mol @ 25°C (gas)	[49]
Heat of formation:	-285.12 @ 25°C (gas)	[10]
	-477. (gas)	[105]
	-493.3 (gas)	[49]
Gibbs (free) energy:	-254.43 kJ/mol @ 25°C (gas)	[10]
	-440. (gas)	[105]
Analytical chemistry: pP <sub>oct</sub> =	2.16	[8], [21], [41]
	2.08	[31]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	304. kPa-m <sup>3</sup> /mol	[41]
	43.1 @ 25°C	[41]
Hydrolysis half-life =	NA	[8]
Electrochemical data:	Unknown	
Clay-organic interaction data:	Unknown	

**Solubility:** Soluble in water, ethanol, ether, acetic acid. [104],[49],[105]  
 0.028 wt% in water @ 25°C [104],[49],[105]  
 9.0 wt% in benzene [10]  
 5.5 wt% in chloroform [10]  
 6.0 wt% in dioxane [10]

**Form:** Colorless gas. Odorless to a faint characteristic ether-like odor at >20 vol%. Shipped as liquified compressed gas. Commercial grades are 99.5% pure. [107],[32],[56]

**Use:** Refrigerant and air conditioner; aerosol propellant; plastics; blowing agent; low-temperature solvent; leak-detecting agent; freezing of food by direct contact; chilling cocktail glasses. [32],[56],[41]

**Fire and explosion hazard:** Very low.

Flash point: NA [107],[105],[49]

UEL: NA

LEL: NA

Autoign. temp.: NA

Nonflammable gas. Dangerous because it emits highly toxic fumes of CO, CO<sub>2</sub>, hydrogen fluoride, hydrogen chloride gas, and phosgene when heated to decomposition. Can react violently with Al. Stable up to 550°C. Use water spray or fog nozzle to keep cylinder cool. Move cylinder away from fire if there is no risk. [32],[107],[108],[55]

**Incompatibility:** Strong oxidizing agents; chemically active metals such as aluminum, magnesium and alloys of more than 2% magnesium, zinc, sodium, potassium, calcium, beryllium, alkali or alkaline earth metals. Silver and copper bearing alloys can act as catalysts for decomposition at high temperatures. The liquid form will attack some forms of plastics, rubber, and coatings. [32],[56],[55]

**Handling:** Avoid heat and flame. Prevent inhalation of gas (appropriate respirator or self-contained breathing apparatus). Prevent contact with skin and eyes (impervious clothing; rubber boots; heavy rubber or neoprene gloves; safety goggles and face shield). Wet clothing should be immediately removed. Use with adequate ventilation (fume hood). Keep container tightly closed. Store in cool, dry, well-ventilated area. Cylinder temperature should not exceed 52°C (125°F). [32],[107],[56],[55]

**Health effects:** Dichlorodifluoromethane is a slight irritant and mild narcotic. Routes of entry are inhalation, and skin or eye contact. Points of attack include central nervous system, skin, and eyes. Exposure may cause dizziness, involuntary trembling, unconsciousness, cardiac arrhythmia, and death. If liquid gets on the skin or eyes it may cause frostbite. It is narcotic in high concentrations. Acute overexposure can cause rapid suffocation. Exposure to high concentrations of vapor may cause light-headedness, disorientation, nausea, vomiting, narcosis, cardiac dysrhythmias, hypotension and death. The cardiac dysrhythmias are potentially lethal because of sensitization of the myocardium to endogenous epinephrine. [32],[56],[55]

## 264 - Dichlorodifluoromethane

### Toxicity: Very low

TWA: 1000 ppm (4950 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: 50000 ppm (247,000 mg/m<sup>3</sup>) [107]

Peak: unknown

Odor threshold: unknown

Carcinogenicity: negative in small animals [36]

Mutagenicity: nonmutagenic [30]

### Exposure:

#### External:

Non-lethal: unknown

Lethal: unknown

#### Oral:

Non-lethal: NA [107]

Lethal: NA [107]

#### Inhalation:

Short-term Inhalation Limits: 5000 ppm (24.7 g/m<sup>3</sup>) for 30 min [107]

Non-lethal: 50,000 ppm (247 g/m<sup>3</sup>) -- dizziness occurs [32]

150,000 ppm (742 g/m<sup>3</sup>) -- unconsciousness [32]

200,000 ppm for 30 min -- systemic eye and CNS effects [51]

Lethal: unknown



1,1-Dichloroethane

 $C_2H_4Cl_2$ 

CAS RN: 75-34-3

Syn: 1,1-Dichloroethane \* Ethane, 1,1-dichloro- \* Asymmetrical  
 dichloroethane \* Chlorinated hydrochloric ether \* Dichlorethane \*  
 Dichloroethane \* Ethylidene chloride \* Ethylidene dichloride \* 1,1-  
 ethylidene dichloride \* NCI-C04535 \* RCRA Waste Number U076 \* UN 2362 (DOT)  
 \*

Molecular formula:  $CH_3CHCl_2$ 

Polychlorinated Aliphatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	98.9598	
Specific gravity:	1.1757	[10], [105]
	1.1755	[49]
	1.174	[51], [107], [104]
Boiling point:	57.30°C	[51], [10], [107], [56], [104], [49]
	57.28°C	[105]
Melting point:	-96.96°C	[49]
	-96.98°C	[105]
	97.0°C	[10]
	-97.4°C	[107], [104]
	-97.7°C	[51]
Refractive index:	1.4164	[10], [49], [105]
Vapor pressure:	5.333 kPa @ -10.2°C	(40mm) [105]
	9.333 @ 0°C	(70mm) [104]
	13.3322 @ 7.2°C	(100mm) [105]
	15.37 @ 10°C	(115.3mm) [41]
	23.998 @ 20°C	(180mm) [104]
	24.26 @ 20°C	(182mm) [32]
	30.36 @ 25°C	(227.7mm) [49]
	30.66 @ 25°C	(230mm) [51]
	31.197 @ 25°C	(234mm) [104]
	35.997 @ 30°C	(270mm) [104]
	53.33 @ 39.8°C	(400mm) [105]
Vapor density:	3.44	[51]
	3.42	[107], [104]
Evaporation rate:	11.6	[32]
Relative dielectric permittivity:	10.0 @ 18°C	[49], [10]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	>0.5882 MOhm-m @ 25°C	[10]
Critical temperature:	250.°C	[49], [10]
	261.5°C	[107]
Critical pressure:	5.07 MPa	[49]
	5.066	[10]
	5.065	[107]
Dynamic viscosity:	0.44 mPa-s @ 20°C	[47]
	0.505 @ 25°C	[49]
	0.430 @ 30°C	[49]
	0.36 @ 40°C	[47]

## 266 - 1,1-Dichloroethane

Kinematic viscosity:	0.37 $\mu\text{m}^2/\text{s}$ @ 20°C	
	0.430 @ 25°C	
	0.366 @ 30°C	
	0.31 @ 40°C	
Surface tension:	24.75 mN/m @ 20°C	[107], [49]
	23.62 @ 30°C	[49]
	23.4 @ 35°C air	[20]
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	6.87x10 <sup>-30</sup> C-m	[105], [10]
	6.07x10 <sup>-30</sup>	[49]
Ionization potential:	11.12 eV (PI)	[105]
Magnetic volume susceptibility:	-8.56 SI @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	7.875 kJ/mol	[10]
	7.870	[49]
Heat of vaporization:	30.5134 kJ/mol	[105]
	30.285	[107]
	29.18	[10]
	28.6 @ bp	[49]
	30.62 @ 25°C	[49]
Heat of sublimation:	30.81 kJ/mol	[10]
Heat capacity @ 25°C:	0.1264 kJ/(mol-K) (liq)	[10]
	0.12627 (liq)	[49]
	0.0764 (gas)	[10]
Heat of combustion:	-1118.3 kJ/mol @ 25°C (liq)	[105]
	-1095.95 (liq)	[49]
	-1098. (liq)	[107]
Heat of formation:	-160.4 kJ/mol @ 25°C (liq)	[10]
	-160.87 (liq)	[49]
	-130.2 (gas)	[10]
	-130.12 (gas)	[49]
Gibbs (free) energy:	-75.78 kJ/mol @ 25°C (liq)	[10]
	-73.35 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	1.79	[8], [21], [31], [24]
	1.78	[41]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	0.595 kPa-m <sup>3</sup> /mol @ 25°C	[41], [24]
	0.955 @ 37°C	[41]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

**Solubility:** Slightly soluble in water. Soluble in acetone, benzene. Very soluble in ethanol, ether. [10]

0.55 wt% in water @ 20°C [104]  
0.51 wt% in water @ 25°C [10]

**Form:** Colorless, oily liquid. Aromatic, ether-like or chloroform-like odor. Chloroform-like or hot saccharine-like taste. [51],[56],[32]

**Use:** Dewaxer of mineral oils; extractant of heat sensitive substances; fumigant; manufacture of vinyl chloride by vapor phase cracking, of high vacuum rubber and silicone grease; chlorinated solvent intermediate; coupling agent in antiknock gasoline; paint, varnish and finish remover; metal degreasing; organic synthesis; ore flotation; formerly used as an anesthetic. [32],[104],[41]

**Fire and explosion hazard:** Very high.

Flash point: (CC) -5.6°C [107],[51]  
(OC) 13.9°C [107]

uel: 11.4% [107]

16% [41]

lel: 5.6% [107],[51]

Autoign. temp.: 458°C [107],[51]

Extremely flammable liquid. Dangerous fire hazard and moderate explosion hazard when exposed to heat or flame. Emits very toxic fumes of HCl, vinyl chloride, phosgene, and CO when heated to decomposition. Fight fire with alcohol or polymer foam, water, CO<sub>2</sub>, dry chemical powder. Water may be ineffective. [32]

**Incompatibility:** Strong oxidizers (may cause fire and explosion); strong caustics (formation of flammable and toxic acetaldehyde gas). Will attack some forms of plastics, rubber, and coatings. [56],[32]

**Handling:** Avoid heat, flame and sources of ignition. Avoid breathing fumes or vapors (appropriate respirator or self-contained breathing apparatus). Avoid repeated or prolonged skin contact (PVA synthetic latex or nitrile gloves; chemical goggles; lab coat). Use with adequate ventilation (fume hood). Keep container tightly closed. Bond and ground containers when transferring liquid. Store in cool, dry, well-ventilated flammable liquid storage area. [56],[107],[32]

**Health effects:** 1,1-Dichloroethane is a mild irritant. Routes of entry are inhalation, ingestion, and eye and skin contact. Points of attack include eyes, skin, liver, lungs, and kidneys. Repeated or prolonged skin contact can produce a slight burn. Vapor may cause irritation of respiratory tract, salivation, sneezing, coughing, dizziness, nausea, vomiting, drowsiness and unconsciousness. There have been no reported cases of human overexposure by inhalation. Chronic exposure may damage the liver, kidneys, and lungs. Splashing the liquid in the eyes may cause irritation, lachrymation and reddening of conjunctiva. Narcotic in high concentrations. There is possible embryotoxicity. [56],[107],[32],[70]

## 268 - 1,1-Dichloroethane

### Toxicity: Very low.

TWA: 200 ppm (810 mg/m<sup>3</sup>) [1]

STEL: 250 ppm (1010 mg/m<sup>3</sup>) [1]

CL: unknown

IDLH: 4000 ppm (16,200 mg/m<sup>3</sup>) [107]

OSHA TWA: 100 ppm (405 mg/m<sup>3</sup>) [51],[56]

Odor threshold: 120-200 ppm (485-810 mg/m<sup>3</sup>) [104],[56]

Carcinogenicity: indefinite [51]

negative in small animals [40]

Mutagenicity: slight [107]

### Exposure:

#### External:

Non-lethal: unknown

Lethal: unknown

#### Oral:

Non-lethal: unknown

Lethal: unknown

#### Inhalation:

Short-term Inhalation Limit: 250 ppm (1010 mg/m<sup>3</sup>) [107]

Non-lethal: unknown

Lethal: unknown

1,2-Dichloroethane

 $C_2H_4Cl_2$ 

CAS RN: 107-06-2

Syn: 1,2-Dichloroethane \* Ethane, 1,2-dichloro- \* 1,2-Bichloridiethane \*  
 1,2-bichloroethane \* Borer sol \* Brocide \* 1,2-DCE \* Destruxol Borer-sol \*  
 Dichloremulsion \* 1,2-Dichlorethane \* Di-chlor-mulsion \*  $\alpha,\beta$ -Dichloroethane  
 \* sym-Dichloroethane \* Dichloroethylene \* Dutch liquid \* Dutch oil \* EDC \*  
 ENT 1656 \* Ethane dichloride \* Ethene dichloride \* Ethylene chloride \*  
 Ethylene dichloride \* 1,2-Ethylene dichloride \* Freon 50 \* Glycol  
 dichloride \* NCI-C00511 \* RCRA Waste Number U077 \* UN 1184 (DOT) \*

Molecular formula:  $ClCH_2-CH_2Cl$ 

Polychlorinated Aliphatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	98.9598		
Specific gravity:	1.253		[107], [10]
	1.25		[104]
	1.2351		[10], [105], [107]
Boiling point:	84.°C		[56]
	83.5°C		[10], [104], [107]
	83.483°C		[49]
	83.47°C		[105]
Melting point:	-35.36°C		[105]
	-35.4°C		[104]
	-35.66°C		[49]
	-35.7°C		[10], [107]
Refractive index:	1.4448		[10], [49], [105]
Vapor pressure:	1.333 kPa @ -13.6°C	(10mm)	[105]
	3.33 @ 0°C	(25mm)	[41]
	5.333 @ 10°C	(40mm)	[104], [105]
	8.13 @ 20°C	(61mm)	[104]
	11.11 @ 20°C	(83.35mm)	[49]
	13.332 @ 29.4°C	(100mm)	[105]
	13.999 @ 30°C	(105mm)	[104]
	53.33 @ 64.0°C	(400mm)	[105]
Vapor density:	3.4		[107]
Evaporation rate:	4.46		[49]
	0.27		[3]
Relative dielectric permittivity:	10.37 @ 25°C		[49]
	10.36 @ 25°C		[10]
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	0.126 W/(m-K) @ 20°C		[105]
Electrical resistivity:	33.3 MOhm-m @ 25°C		[10]
Critical temperature:	288.4°C		[47]
	288.°C		[49], [10], [107]
Critical pressure:	5.4 MPa		[49]
	5.370		[10], [47]
	5.1		[107]

## 270 - 1,2-Dichloroethane

Dynamic viscosity:	1.077 mPa-s @ 0°C	[105]
	0.887 @ 15°C	[10], [49]
	0.800 @ 19.4°C	[105]
	0.730 @ 30°C	[49]
	0.652 @ 40°C	[105]
	0.565 @ 50°C	[105]
	0.479 @ 70°C	[105]
Kinematic viscosity:	0.860 $\mu\text{m}^2/\text{s}$ @ 0°C	
	0.708 @ 15°C	
	0.638 @ 19.4°C	
	0.583 @ 30°C	
	0.520 @ 40°C	
	0.451 @ 50°C	
	0.382 @ 70°C	
Surface tension:	24.15 mN/m @ 20°C air	[20]
	32.2 @ 20°C	[107]
	32.23 @ 20°C	[49]
	32.48 @ 20°C	[15]
	31.06 @ 30°C	[15]
	30.84 @ 30°C	[49]
	28.27 @ 40°C	[15]
Contact angle:	unknown	
Thermal expansion coefficient:	0.001141 K-1 @ 20°C	[49]
	0.00121 @ 55°C	[49]
Compressibility:	0.691 nPa-1 @ 0°C	[105]
	0.742 @ 10°C	[105]
	0.797 @ 20°C	[105]
	0.846 @ 30°C	[49]
	0.858 @ 30°C	[105]
	0.925 @ 40°C	[105]
Vapor diffusivity:	unknown	
Solution diffusivity:	2.8 $\text{nm}^2/\text{s}$ in Benzene	[47]
Electric dipole moment:	6.104x10 <sup>-30</sup> C-m	[49]
	4.003	[10]
Ionization potential:	11.12 eV (PI)	[105]
Magnetic volume susceptibility:	-9.51x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	8.843 kJ/mol	[10]
	8.837	[49]
	8.833	[105]
	8.75	[105], [107]
	33.288 kJ/mol	[105]
Heat of vaporization:	32.03	[10]
	32.02	[49]
	31.7	[107]
	35.46 kJ/mol	[10]
Heat of sublimation:	0.1294 kJ/(mol-K) (liq)	[10], [105]
	0.12899 (liq)	[49]
	0.0787 (gas)	[10], [105]
Heat of combustion:	-1111.48 kJ/mol @ 25°C (liq)	[49]
	-1135. (gas)	[105]

Heat of formation:	-165.3	kJ/mol @ 25°C	(liq)	[10],[105]
	-169.66		(liq)	[49]
	-129.8		(gas)	[10],[105]
	-126.78		(gas)	[49]
Gibbs (free) energy:	-79.68	kJ/mol @ 25°C	(liq)	[10],[105]
	-73.90		(gas)	[10]
	-73.98		(gas)	[105]
Analytical chemistry: $pP_{oct}$ =	1.48			[8],[21],[31],[41],[24]
	1.45			[4],[27]
	$pK_s$ =	unknown		
	$pK_a$ =	unknown		
	$pK_{BH}$ =	3.44		[49]
Henry's law constant =	0.0997	kPa-m <sup>3</sup> /mol @ 25°C		[41]
	0.0990			[24]
	0.133		@ 25°C	[41]
	0.255		@ 37°C	[41]
Hydrolysis half-life =	NA			[8]

Electrochemical data: Unknown

Clay-organic interaction data: Karickhoff (1981), Rao et al. (1988).

Solubility: Slightly soluble in water. Soluble in acetone, benzene.

Miscible with ethanol, ether, chloroform, mineral oil. [10],[49],[104]

0.81	wt% in water @ 20°C	[10],[49]
0.869	wt% in water @ 20°C	[104]
0.92	wt% in water @ 30°C	[104]

Form: Colorless liquid. Sweet chloroform-like or ether-like odor. Sweet taste. [56],[104]

Use: Solvent for fats, oils, waxes, gums, resins, asphalts, bitumen, cellulose acetate, cellulose ester, paint, and particularly for rubber; manufacture of acetyl cellulose, tobacco extract, ethylene glycol, diaminoethylene, polyvinyl chloride, nylon, viscose rayon, styrene-butadiene rubber, various plastics; intermediate insecticidal fumigant (peach tree borer, Japanese beetle, toot-knot nematode); degreaser in engineering, textile and petroleum industries; soaps and scouring compounds; wetting and penetrating agents; extracting agent for soybean oil, caffeine, spices (annatto, paprika, turmeric); pickling agent; ingredient in cosmetics (nail lacquers); dry-cleaning agent; lead scavenger in antiknock unleaded gasoline; ore flotation. 17th highest volume chemical produced in U.S. (1979). [56],[104],[41]

Fire and explosion hazard: High

Flash point: (CC) 12.8°C [107]

(CC) 13°C [49]

(OC) 15.5°C [107]

uel: 15.6% [107]

15.9% [51]

lel: 6.2% [107],[51]

Autoign. temp.: 413°C [107]

## 272 - 1,2-Dichloroethane

Highly flammable liquid. Burns with a smokey flame. Relatively low flash points. Dangerous fire hazard when exposed to heat or flame. Flashback along vapor trail may occur. Moderate explosion hazard in the form of vapor when exposed to flame. Can react vigorously with oxidizing materials. When heated to decomposition it emits highly toxic fumes of phosgene and hydrogen chloride gas. Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder. Water may be ineffective. [107],[55]

**Incompatibility:** Dinitrogen tetroxide; chemically active metals such as aluminum and magnesium powder; strong oxidizers; strong caustics; sodium; potassium. [51],[56],[55]

**Handling:** Keep away from heat, sparks and flame. Avoid breathing vapor or mist (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, on clothing (PVA synthetic latex or nitrile gloves; lab coat; chemical goggles or face shield). Use in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Bond and ground containers when transferring liquid. Store under nitrogen. Store in cool, dry, well-ventilated flammable liquid storage area. [107],[56],[55]

**Health effects:** 1,2-Dichloroethane is an poison and carcinogen. Routes of entry are inhalation of vapor, ingestion of liquid, skin absorption, and eye and skin contact. Points of attack include skin, eyes, liver, respiratory system, central nervous system, and kidneys. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Prolonged exposure can cause nausea, headache and vomiting, damage to the liver, gastrointestinal disturbances, damage to the kidneys. It may also cause drowsiness, equilibrium disturbances, narcosis, and abdominal cramps. The liquid may cause serious damage to the eyes including corneal clouding. Dermatitis may follow repeated skin contact. Chronic effects of over exposure may include liver and kidney damage, cardiovascular effects, and mutagenicity. Listed as a carcinogen by the EPA. [56],[107],[55],[71]

**Toxicity:** Moderate

TWA: 10 ppm (40 mg/m<sup>3</sup>) [1]

STEL no value set [1]

CL: 100 ppm (405 mg/m<sup>3</sup>) [56]

IDLH: 1000 ppm (4050 mg/m<sup>3</sup>) [107],[56]

Peak: 200 ppm (810 mg/m<sup>3</sup>) for 5 min in any 3-hr period [107],[56]

Odor threshold: 100 ppm (405 mg/m<sup>3</sup>) [107]

20-40 ppm (80-160 mg/m<sup>3</sup>) -- detection [104]

20-140 ppm ( 80-570 mg/m<sup>3</sup>) -- recognition [104]

Carcinogenicity: probable [104]

limited evidence [55],[40]

Mutagenicity: suspected [104]



**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: 286 mg/kg [55]

714 mg/kg -- adult male [55]

Inhalation:

Short-term Inhalation Limit: 200 ppm for 5 min over 3-hr period [107]

Non-lethal: >50 ppm (200 mg/m<sup>3</sup>) -- unsatisfactory [104]

100 ppm (405 mg/m<sup>3</sup>) -- symptoms of illness occur [104]

500 ppm for 60 min -- severe toxic effects [104]

Lethal: unknown

## 274 - 1,1-Dichloroethene

1,1-Dichloroethene

 $C_2H_2Cl_2$ 

CAS RN: 75-35-4

Syn: 1,1-Dichloroethene \* Ethene, 1,1-dichloro- \* asym-dichloroethylene \*  
 1,1-DCE \* 1,1-dichloroethylene \* Ethylene, 1,1-dichloro- \* NCI-C54262 \*  
 RCRA Waste Number U078 \* UN 1303 (DOT) \* unsym-Dichloroethylene \* VC \* VDC  
 \* Vinylidene chloride \* Vinylidene chloride II \* Vinylidene chloride,  
 inhibited \* Vinylidene dichloride \* Vinylidine dichloride \*

Molecular formula:  $CH_2=CCl_2$ 

Polychlorinated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	96.9439	
Specific gravity:	1.218	[105], [104]
	1.213	[51]
	1.213229	[49]
	1.2129	[10]
	1.21	[107]
Boiling point:	37.°C	[105]
	31.9°C	[104]
	31.7°C	[56]
	31.6°C	[10], [51], [107]
	31.56°C	[49]
Melting point:	-122.°C	[51], [107]
	-122.1°C	[105]
	-122.5°C	[104]
	-122.56°C	[49]
	122.6°C	[10]
Refractive index:	1.4249	[105]
	1.4247	[10]
	1.42468	[49]
Vapor pressure:	5.333 kPa @ -31.1°C	(40mm) [105]
	10.66 @ -20°C	(80mm) [41]
	13.33 @ -15°C	(100mm) [105]
	18.00 @ -10°C	(135mm) [41]
	28.66 @ 0°C	(215mm) [41]
	53.33 @ 14.8°C	(400mm) [105]
	66.661 @ 20°C	(500mm) [104]
	78.793 @ 25°C	(591mm) [104], [23]
	79.86 @ 25°C	(599mm) [49]
Vapor density:	95.99 @ 30°C	(720mm) [104]
	3.25	[104]
	3.3	[107]
Evaporation rate:	unknown	
Relative dielectric permittivity:	4.67 @ 16°C	[105]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	222.°C	[49]
	271.°C	[10]
Critical pressure:	5.20 MPa	[49]
Dynamic viscosity:	0.422 mPa-s @ 0°C	[49]
	0.358 @ 20°C	[49]

Kinematic viscosity:	0.348 $\mu\text{m}^2/\text{s}$ @ 0°C	
	0.295 @ 20°C	
Surface tension:	24. mN/m @ 15°C	[107]
Contact angle:	unknown	
Thermal expansion coefficient:	NA	
Compressibility:	unknown	
Vapor diffusivity:	9.4 $\mu\text{m}^2/\text{s}$ (calc)	[59]
Solution diffusivity:	0.95 $\text{nm}^2/\text{s}$ (calc)	[59]
Electric dipole moment:	4.336x10 <sup>-30</sup> C-m	[10]
	4.470	[105]
	4.27	[49]
Ionization potential:	9.65 eV (PI)	[105]
Magnetic volume susceptibility:	-7.98x10 <sup>-6</sup> SI units @ 15°C	[105]
Speed of sound:	unknown	
Heat of melting:	6.519 kJ/mol	[10]
	6.514	[49]
Heat of vaporization:	26.209 kJ/mol	[10]
	29.083	[107]
	30.1944	[105]
	26.18 @ bp	[49]
	26.48 @ 25°C	[49]
Heat of sublimation:	26.49 kJ/mol	[10]
Heat capacity @ 25°C:	0.113 kJ/(mol-K) (liq)	[105]
	0.1114 (liq)	[10]
	0.0673 (gas)	[105]
	0.06707 (gas)	[10]
@ 25.15°C:	0.11190 (liq)	[49]
Heat of combustion:	-1095.95 kJ/mol @ 25°C (liq)	[49]
	-1095.46	[107]
Heat of formation:	-24.28 kJ/mol @ 25°C (liq)	[10]
	-24.31 (liq)	[49]
	1.256 (gas)	[10]
	2.43 (gas)	[49]
Gibbs (free) energy:	24.49 kJ/mol @ 25°C (liq)	[10]
	24.20 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	2.13	[31], [41], [59]
	1.84	[72]
	1.48	[8], [41]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	19.3 kPa-m <sup>3</sup> /mol	[41]
	2.13	[41]
	1.52	[41]
	6.4 dimensionless	[59]
Hydrolysis half-life =	<3.0x10 <sup>7</sup> sec	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

## 276 - 1,1-Dichloroethene

**Solubility:** Practically insoluble in water. Soluble in ethanol, acetone, benzene and other organic solvents. Very soluble in chloroform, ether. [10]

0.021 wt% in water	[10]
0.021 wt% in water @ 25°C	[49]
0.04 wt% in water	[59]

**Form:** Colorless liquid. Mild, sweet, chloroform-like odor. Commercial grades contain 0.02% of monomethylether of hydroquinone as a polymerization inhibitor. [56],[104]

**Use:** Intermediate in the production of "vinylidene polymer plastics" such as Saran® and Velon® (used in screens, upholstery, fabrics, carpets, etc.); adhesives; synthetic fibers; copolymerized with vinyl chloride or acrylonitrile to form various kinds of saran; manufacture of 1,1,1-trichloroethane. [56],[104]

**Fire and explosion hazard:** Very high.

Flash point: (OC) -17.8°C [107],[51]

(OC) -10°C [49]

uel: 16.0% [107],[51]

15.5% [41]

lel: 7.3% [107],[51]

6.5% [41]

Autoign. temp.: 513°-555°C [107]

570°C [51]

Extremely flammable liquid. Highly volatile. Flashback along vapor trail may occur. Moderate explosion hazard when in the form of gas and exposed to heat or flame. Can explode spontaneously. Emits highly toxic fumes of hydrogen chloride, CO, and phosgene. Reacts violently with chlorosulfonic acid, HNO<sub>3</sub>, oleum. Can react vigorously with oxidizing materials. Polymerizes to a plastic at temperatures above 0°C and especially in the presence of sunlight, air, copper, aluminum, or heat. Uncontrolled polymerization may lead to explosive reaction products with oxygen or ozone. Several inhibitors to preserve the monomer have been invented (eg., 200 ppm methyl ether of hydroquinone, 0.6%-0.8% phenol). Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder. Water may be ineffective. [51],[107]

**Incompatibility:** Oxidizing materials; air; chlorotrifluoroethylene; ozone; perchloryl fluoride; chlorosulfonic acid; HNO<sub>3</sub>; oleum; copper, aluminum; and their alloys. [51],[107]

**Handling:** Do not expose to air, heat, sparks or flame. Avoid breathing vapors (appropriate respirator or self-contained breathing apparatus). Prevent skin contact (rubber gloves and boots, goggles or face shield, lab coat). Use with adequate ventilation (fume hood). Keep container tightly closed. Bond and ground containers when transferring liquid. Store under nitrogen. Refrigerate. Store in cool, dry, well-ventilated, flammable liquid storage area or cabinet. [56],[107]

**Health effects:** 1,1-Dichloroethene is an irritant, narcotic, and potential carcinogen. Routes of entry are inhalation, ingestion, and skin absorption. Points of attack include liver, eyes, skin, and respiratory system. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract after just a few minutes of contact. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. It is narcotic in high concentrations. Chronic effects to overexposure may include liver and/or kidney damage, and cardiovascular effects. It has moderate carcinogenic potential. [56],[107],[55],[72]

**Toxicity:** High.

TWA: 5 ppm (20 mg/m<sup>3</sup>) [1] (NIOSH recommends 1 ppm [56])

STEL: 20 ppm (80 mg/m<sup>3</sup>) [1],[56]

CL: 5 ppm (20 mg/m<sup>3</sup>) over any 15 minute period [51]

IDLH: unknown

Peak: unknown

Odor threshold: 500 ppm (2000 mg/m<sup>3</sup>) [104]

Carcinogenicity: suspected [56]

negative in small animals [26]

probable [72]

Mutagenicity: probable [51]

positive [9]

**Exposure:**

**External:**

Non-lethal: unknown

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: unknown

**Inhalation:**

Short-term Inhalation Limit: unknown

Non-lethal: 25 ppm (100 mg/m<sup>3</sup>) -- liver and kidney damage [107]

Lethal: unknown

278 - *trans*-1,2-Dichloroethene*trans*-1,2-DichloroetheneC<sub>2</sub>H<sub>2</sub>Cl<sub>2</sub>

CAS RN: 156-60-5

Syn: *trans*-1,2-Dichloroethene \* Ethene, 1,2-dichloro-, (E)- \* *trans*-Acetylene dichloride \* 1,2-Dichloroethene \* (E)-1,2-Dichloroethene \* Dichloroethylene \* 1,2-Dichloroethylene \* *trans*-Dichloroethylene \* *trans*-1,2-Dichloroethylene \* Dioform \* RCRA Waste Number U079 \*

Molecular formula: ClCH=CHCl

Polychlorinated Unsaturated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	96.9439	
Specific gravity:	1.2565	[105], [106]
	1.2547	[49]
	1.2546	[10]
	1.257	[22]
	1.26	[104]
Boiling point:	47.°-49°C	[22]
	47.67°C	[49]
	47.5°C	[106], [105]
	47.7°C	[10]
	48.°C	[104]
	48.4°C	[47]
Melting point:	-49.8°C	[10], [49]
	-50.°C	[106], [47], [105], [104]
Refractive index:	1.4454	[106], [105]
	1.4462	[10], [49]
Vapor pressure:	5.33 kPa @ -17.0°C (40mm)	[105]
	8.00 @ -10.0°C (60mm)	[47], [20]
	13.33 @ -0.2°C (100mm)	[105]
	26.66 @ 14.3°C (200mm)	[104]
	35.33 @ 20°C (265mm)	[32]
	45.3 @ 25°C (340mm)	[49]
	53.33 @ 30.8°C (400mm)	[105]
Vapor density:	3.34	[104]
Evaporation rate:	unknown	
Relative dielectric permittivity:	2.1 @ 25°C	[11]
	2.14 @ 25°C	[10], [49], [105]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	243.3°C	[10], [49]
Critical pressure:	5.51 MPa	[10], [49]
Dynamic viscosity:	0.423 mPa·s @ 15°C	[49]
	0.404 @ 20°C	[10], [49]
Kinematic viscosity:	0.337 μm <sup>2</sup> /s @ 15°C	
	0.322 @ 20°C	
Surface tension:	25. mN/m @ 20°C	[49], [10]
Contact angle:	unknown	
Thermal expansion coefficient:	0.00136 K <sup>-1</sup> @ 15°-45°C	[49]
Compressibility:	1.119 nPa <sup>-1</sup> @ 25°C	[105]
Vapor diffusivity:	9.7 μm <sup>2</sup> /s (calc)	[59]
Solution diffusivity:	0.95 nm <sup>2</sup> /s (calc)	[59]

Electric dipole moment:	2.3x10 <sup>-30</sup> C-m	[49]
Ionization potential:	9.64 eV (PI)	[105]
Magnetic volume susceptibility:	-8.02x10 <sup>-6</sup> SI units @ 15°C	[105]
Speed of sound:	unknown	
Heat of melting:	7.20 kJ/mol	[10]
	11.98	[49]
Heat of vaporization:	27.8 kJ/mol	[10]
	28.89	[49]
	30.33	[105]
Heat of sublimation:	28.9 kJ/mol	[10]
Heat capacity @ 25°C:	0.11276 kJ/(mol-K) (liq)	[49]
	0.1130 (liq)	[105]
	0.06670 (gas)	[10]
Heat of combustion:	-1092.28 kJ/mol @ 25°C (liq)	[49]
Heat of formation:	-23.14 kJ/mol @ 25°C (liq)	[49]
	-23.15 (liq)	[105]
	4.187 (gas)	[10]
	6.15 (gas)	[49]
Gibbs (free) energy:	27.30 kJ/mol @ 25°C (liq)	[105]
	26.59 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	2.09	[31], [41]
	2.06	[24]
	1.48	[8], [59]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	38.9 kPa-m <sup>3</sup> /mol	[41]
	0.73	[41]
	0.681	[24]
	0.539	[41]
	0.683 @ 25°C	[41]
	1.226 @ 37°C	[41]
	1.77 dimensionless	[59]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Rao et al. (1988).

Solubility: Slightly soluble in water. Very soluble in benzene, chloroform. Miscible with ethanol, ether, acetone, most organic solvents. [10], [105], [22], [104], [41]

0.63 wt% in water @ 20°C	[10]
0.6 wt% in water @ 20°C	[14], [104]
0.63 wt% in water @ 25°C	[49], [47]

Form: Colorless liquid with an ethereal, slightly acrid, pleasant, chloroform-like odor. Decomposes slowly on exposure to air, light, and moisture. [107], [22]

## 280 - *trans*-1,2-Dichloroethene

**Use:** Solvent for waxes, resins, and acetylcellulose; extraction of rubber; refrigerant; manufacture of pharmaceuticals and artificial pearls; extraction of oils and fats from fish and meat; low temperature solvent for heat sensitive solutions (eg. caffeine); constituent of perfumes and thermoplastics; organic synthesis. [56],[104],[22]

**Fire and explosion hazard:** High.

Flash point: (CC) 2.8°C [107]

(CC) 2.0°C [51]

(OC) 4°C [49]

(OC) 2.8°C [107]

(OC) 2.0°C [51]

UEL: 12.8% [51],[49],[107]

LEL: 9.7% [51],[49],[107]

Autoign. temp.: 460°C [107]

Highly flammable liquid. Phosgene, CO, and hydrogen chloride fumes may form in fires. Flash back along vapor trail can occur. Fight fire with water spray, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. Water may be ineffective. [51],[107],[55]

**Incompatibility:** Alkalies; difluoromethylene dihypofluorite; nitrogen tetroxide; strong oxidizers. May decompose on exposure to air, moisture, and light. [51],[107],[55]

**Handling:** Keep away from heat, sparks, and open flame. Do not breathe vapor (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (chemical resistant gloves, safety goggles, other protective clothing. Use with adequate ventilation (fume hood). Employees should wash promptly when skin is wet or contaminated. Remove clothing promptly if wet or contaminated to avoid flammability hazard. Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, flammable liquid storage area or cabinet. [56],[55]

**Health effects:** Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include respiratory system, eyes, skin, and central nervous system. Vapor or mist is irritating to the eyes, skin, mucous membranes, and upper respiratory tract. Inhalation may cause nausea, vomiting, weakness, epigastric cramps, tremor, central nervous system depression. Ingestion causes slight depression to deep narcosis. [107],[55],[73]

**Toxicity:** Low

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: 4000 ppm (15,860 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: unknown

Carcinogenicity: unknown

Mutagenicity: laboratory experiments have shown mutagenic effects [55]  
nonmutagenic in Salmonella strains [73]

**Exposure:** Unknown



Dichloromethane

 $\text{CH}_2\text{Cl}_2$ 

CAS RN: 75-09-2

Syn: Dichloromethane \* Methane, dichloro- \* Aerothene MM \* DCM \* Freon 30  
 \* Methane dichloride \* Methylene bichloride \* Methylene chloride (DOT) \*  
 Methylene dichloride \* Narkotil \* NCI-C50102 \* R 30 \* RCRA Waste Number  
 U080 \* Solaesthin \* Solmethine \* UN 1593 (DOT) \*

Molecular formula:  $\text{CH}_2\text{Cl}_2$ 

Polychlorinated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	84.9329	
Specific gravity:	1.3	[32]
	1.336	[47], [48]
	1.3266	[105], [106]
	1.326	[51]
	1.3256	[49]
	1.3255	[10], [108], [16]
	1.322	[107]
Boiling point:	40.5°C	[10]
	40.1°C	[22]
	40.°C	[105], [56], [106], [48]
	40.°-41°C	[47]
	40.°-42°C	[104]
	39.75°C	[108], [16]
	39.8°C	[51], [107], [32]
	39.64°C	[49]
Melting point:	-94.92°C	[49]
	-95.1°C	[105], [106]
	-95.14°C	[16]
	-96.5°C	[48]
	-96.7°C	[10], [51], [107], [47]
	-97.°C	[104], [32], [22]
Refractive index:	1.4242	[105], [106], [16]
	1.4244	[108], [22]
	1.42416	[49]
	1.4246	[10]
Vapor pressure:	5.33 kPa @ -22.3°C (40mm)	[47], [105]
	8.00 @ -15.7°C (60mm)	[47]
	13.33 @ -6.3°C (100mm)	[105], [47]
	19.65 @ 0°C (147.4mm)	[41]
	26.66 @ 8.0°C (200mm)	[47]
	30.62 @ 10°C (229.7mm)	[41]
	46.53 @ 20°C (349mm)	[104]
	46.66 @ 20°C (350mm)	[32]
	50.7 @ 22°C (380mm)	[51]
	53.33 @ 24.1°C (400mm)	[47], [105]
	58.10 @ 25°C (435.8mm)	[49], [16]
	66.66 @ 30°C (500mm)	[104]
Vapor density:	2.93	[104], [51]
	2.9	[107], [32]
Evaporation rate:	27.5	[32]
	14.5	[49], [3]

## 282 - Dichloromethane

Relative dielectric permittivity:	10.27 @ -8.6°C	[2]
	9.1 @ 18°C	[11]
	9.08 @ 20°C	[10], [105]
	8.9 @ 22.0°C	[2]
	8.93 @ 25°C	[49]
	8.93 @ 28.4°C	[2]
	8.649 @ 30°C	[49]
	8.47 @ 32.8°C	[2]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.162 W/(m-K) @ -20°C	[48]
	0.159 @ -10°C	[48]
	0.158 @ 0°C	[48]
	0.122 @ 0°C	[105]
	0.111 @ 5°C	[47]
	0.155 @ 20°C	[48]
	0.96 @ 86°C	[47]
Electrical resistivity:	232.6 MOhm-m @ 25°C	[11]
Critical temperature:	237.34°C	[14]
	237.°C	[49], [105], [47], [10]
	245.°C	[107], [48]
Critical pressure:	6.076 MPa	[14]
	6.08	[105], [47], [10]
	6.17	[49], [107]
Dynamic viscosity:	0.68 mPa-s @ -20°C	[48]
	0.602 @ -10°C	[48]
	0.537 @ 0°C	[48]
	0.481 @ 10°C	[48]
	0.449 @ 15°C	[10], [105], [49]
	0.435 @ 20°C	[48]
	0.430 @ 20°C	[22]
	0.4043 @ 27.61°C	[49]
	0.396 @ 30°C	[48]
	0.393 @ 30°C	[105], [49]
Kinematic viscosity:	0.51 $\mu\text{m}^2/\text{s}$ @ -20°C	
	0.454 @ -10°C	
	0.405 @ 0°C	
	0.363 @ 10°C	
	0.338 @ 15°C	
	0.328 @ 20°C	
	0.324 @ 20°C	
	0.3040 @ 27.61°C	
	0.299 @ 30°C	
	0.296 @ 30°C	
Surface tension:	28.00 mN/m @ 20°C	[16]
	27.89 @ 20°C	[49]
	26.52 @ 20°C (air)	[105]
	26.54 @ 30°C	[49]
	26.41 @ 30°C	[16]
Contact angle:	unknown	
Thermal expansion coefficient:	0.001391 K <sup>-1</sup>	[49]
Compressibility:	0.974 nPa <sup>-1</sup> @ 25°C	[105]
	1.026 @ 25°C	[49]
Vapor diffusivity:	10.4 $\mu\text{m}^2/\text{s}$ @ 25°C	[59]

Solution diffusivity:	0.11 nm <sup>2</sup> /s (calc)	[59]
Electric dipole moment:	5.337x10 <sup>-30</sup> C-m	[105], [10]
	3.80x10 <sup>-30</sup>	[49]
Ionization potential:	11.35 eV (PI)	[105]
Magnetic volume susceptibility:	-9.21x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	6.160 kJ/mol	[49]
	6.006	[107]
	6.002	[105]
	4.6	[10]
Heat of vaporization:	27.98 kJ/mol	[49]
	27.73	[16]
	28.027	[107]
	28.092	[48]
	28.2	[10]
	31.7037	[105]
Heat of sublimation:	29.1 kJ/mol	[10]
Heat capacity @ 25°C:	0.1001 kJ/(mol-K) (liq)	[108], [105]
	0.0512 (gas)	[108], [105]
	0.05091 (gas)	[10]
Heat of combustion:	-557.89 kJ/mol @ 25°C (liq)	[49]
	-558.3 (liq)	[20]
	-587.3 (gas)	[20]
	-447.2 @ 20°C (gas)	[105]
Heat of formation:	-124.3 kJ/mol @ 25°C (liq)	[10]
	-121.54 (liq)	[105]
	-121.50 (liq)	[20]
	-121.46 (liq)	[49]
	-95.46 (gas)	[10]
	-95.40 (gas)	[49]
	-92.53 (gas)	[105]
	-92.52 (gas)	[20]
Gibbs (free) energy:	-70.46 kJ/mol @ 25°C (liq)	[10]
	-67.37 (liq)	[105]
	-68.92 (gas)	[10]
	-65.94 (gas)	[105]
Analytical chemistry: pP <sub>oct</sub> =	1.30	[41]
	1.26	[31]
	1.25	[8], [21], [24], [41], [59]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	0.289 kPa-m <sup>3</sup> /mol	[24]
	0.203 - 0.358	[41]
	0.130 dimensionless	[59]
Hydrolysis half-life =	2.2x10 <sup>10</sup> sec	[13]
	4.7x10 <sup>7</sup> to 2.2x10 <sup>10</sup> sec	[8]

Electrochemical data: Wawzonek and Duty (1961), Meites and Zuman (1977), Meites et al. (1977a), Ebersson and Utley (1983b).

Clay-organic interaction data: Unknown

## 284 - Dichloromethane

**Solubility:** Slightly soluble in water. Miscible with ethanol, ether.  
[47],[10],[105],[32],[108],[49]

1.32 wt% in water @ 20°C	[108],[32]
2.0 wt% in water @ 20°C	[10],[47],[104]
1.67 wt% in water @ 25°C	[104]
1.30 wt% in water @ 25°C	[49]

**Form:** Colorless, volatile liquid. Pleasant, penetrating, ether-like or chloroform-like odor. [51],[32],[107],[22]

**Use:** Solvent for cellulose acetate; degreasing and cleaning fluids; as solvent in food processing; plastics; paint removers; propellants; blowing agent in foams; manufacture of aerosols, photographic film, synthetic fibers; extraction of naturally-occurring heat sensitive substances; textile and leather coatings; pharmaceutical; spotting agent; dewaxing; organic synthesis. [56],[104],[108],[22]

**Fire and explosion hazard:** Very low

Flash point: none with normal testing methods [32],[49]

uel: 19% (at elevated temperatures) [32],[107]

66.4% in O<sub>2</sub> [51]

lel: 12% (at elevated temperatures) [32],[107]

15.5% in O<sub>2</sub> [51],[49]

Autoign. temp.: 556°C [32]

615°C [51]

640°C [107]

642°C [49]

662°C [22]

**Nonflammable gas.** Volatile. Vapor is not flammable and when mixed with air is not explosive under conditions likely to be encountered. Not an explosion hazard under ordinary conditions. Dangerous when heated to decomposition as it emits highly toxic fumes of phosgene, hydrogen chloride, and carbon monoxide. Fight fire with dry chemical, CO<sub>2</sub>, alcohol or polymer foam. [51],[32]

**Incompatibility:** Strong oxidizers; heat; strong caustics; chemically active metals such as aluminum or magnesium powder, sodium and potassium; Li; NaK; potassium-tert-butoxide; (KOH + n-methyl-n-nitrosourea). Will attack some forms of plastics, rubber, and coatings. [51],[32],[56]

**Handling:** Avoid heat and sunlight. Avoid inhalation (appropriate respirator or self-contained breathing apparatus). Avoid skin contact (PVA synthetic latex or neoprene gloves, goggles and face shield, lab coat and apron). Safety showers and eye bath should be provided. Use in well-ventilated area (fume hood). Keep container tightly closed. Store in secure poison area. Keep container out of sun and away from heat.  
[57],[56],[53]

**Health effects:** Dichloromethane is an irritant and mild narcotic. Routes of entry are inhalation of vapors, percutaneous absorption of the liquid, ingestion, and eye and skin contact. Points of attack include skin, eyes, cardiovascular system, liver, respiratory system, and central nervous system. It is irritating to the eyes, mucous membranes, and upper respiratory tract at high concentrations. Except for its property of

inducing narcosis, it has very few other acute toxic effects. Its narcotic powers are quite strong, and in view of its great volatility, care should be taken in its use. Can cause dermatitis upon prolonged skin contact. Inhalation of vapors may cause nausea, vomiting, light-headedness or headache. Chronic exposure may result in liver and/or kidney damage. May cause embryotoxicity. [32],[51],[107],[56],[81]

**Toxicity:** Low

TWA: 50 ppm (175 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: 1000 ppm (3.5 g/m<sup>3</sup>) [51],[56],[32]

IDLH: 5000 ppm (17.4 g/m<sup>3</sup>) [107],[56]

Peak: 2000 ppm (7 g/m<sup>3</sup>) for 5 min duration in 2 hr period [51],[56],[32]

NIOSH recommends TWA=75 ppm (260 mg/m<sup>3</sup>) and CL=500 ppm (1750 mg/m<sup>3</sup>) [51]

Odor threshold: 205-307 ppm (712-1065 mg/m<sup>3</sup>) [107]

300 ppm (1.04 g/m<sup>3</sup>) [56]

25-320 ppm (85-1110 mg/m<sup>3</sup>) [32]

1.15-11.5 ppm (4-40 mg/m<sup>3</sup>) -- detection [104]

58-580 ppm (200-2000 mg/m<sup>3</sup>) -- recognition [104]

Carcinogenicity: suspected human carcinogen [1],[56]

clear evidence in small animals [26],[38]

Mutagenicity: experimental equivocal tumorigenic agent [51],[33]  
positive [30]

**Exposure:**

**External:**

Non-lethal: 7200 ppm (25 g/m<sup>3</sup>) for 20 min -- eye irritation [51]

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: 0.5 to 5 g/kg body wt -- 50% chance of death [107]

0.357 g/kg [55]

**Inhalation:**

Short-term Inhalation Limits: 500 ppm (1750 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: 500 ppm in 1 yr at intervals -- CNS effects [51]

500 ppm (1750 mg/m<sup>3</sup>) for 8 hr -- effects on all blood elements [51]

500-1000 ppm (1750-3500 mg/m<sup>3</sup>) for 1-2 hr -- light-headedness  
and sustained elevation of carboxyhemoglobin level [32]

2300 ppm (7990 mg/m<sup>3</sup>) for 30 min -- nausea [51]

7200 ppm for 8 min -- parasthesia of the extremities [51]

7200 ppm for 16 min -- pulse acceleration to 100 [51]

7200 ppm for 20 min -- congestion in the head and sense of heat [51]

25000 ppm (86.8 g/m<sup>3</sup>) for 2 hr -- non-lethal [51]

Lethal: unknown

## 286 - 2,4-Dichlorophenol

2,4-Dichlorophenol

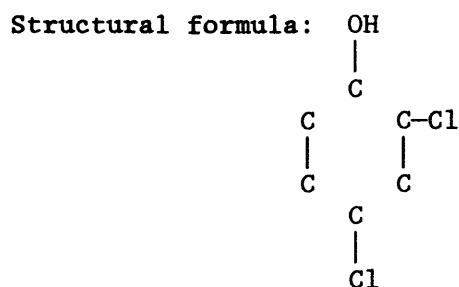
 $C_6H_4Cl_2O$ 

CAS RN: 120-83-2

Syn: 2,4-Dichlorophenol \* Phenol, 2,4-dichloro- \* 3-Chloro-4-hydroxychlorobenzene \* DCP \* 2,4-DCP \* 2,4-Dichlorohydroxybenzene \* 4,6-Dichlorohydroxybenzene \* 4,6-Dichlorophenol \* NCI-C55345 \* RCRA Waste Number U081 \*

Molecular formula: 2,4- $C_6H_3Cl_2OH$ 

Polychlorinated Phenol



## Physical properties:

Relative molecular mass:	163.003	
Specific gravity:	1.383 @ 60/25	[104],[51],[47],[10]
	1.4 @ 15°C (solid)	[107]
Boiling point:	209.°-210°C	[47],[10]
	210.°C	[51],[106],[105],[56],[104],[22]
	216.°C	[107]
Melting point:	45.°C	[51],[47],[105],[107],[56],[104]
	42.°-43°C	[10]
Refractive index:	unknown	
Vapor pressure:	0.016 kPa @ 20°C	(0.12mm) [41]
	0.008 @ 20°C	(0.59mm) [31]
	0.133 @ 53.0°C	(1mm) [51],[47],[105]
	1.333 @ 92.8°C	(10mm) [105]
Vapor density:	5.62	[51]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	unknown	
Kinematic viscosity:	unknown	
Surface tension:	unknown	
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	20.091 kJ/mol	[105]

Heat of vaporization: 55.3930 kJ/mol [105]  
 Heat of sublimation: unknown  
 Heat capacity @ 25°C: unknown  
 Heat of combustion: unknown  
 Heat of formation: unknown  
 Gibbs (free) energy: unknown

Analytical chemistry:  $pP_{oct}$  = 3.30 [21]  
 3.08 [27],[21]  
 3.06 [21],[41]  
 2.90 [31]  
 2.75 [8]  
 $pK_s$  = unknown  
 $pK_a$  = 7.85 @ 25°C [10],[11],[31]  
 $pK_{BH}$  = unknown  
 Henry's law constant =  $6.75 \times 10^{-4}$  atm-m<sup>3</sup>/mol (calc) [41]  
 $3.27 \times 10^{-4}$  (est) [41]  
 Hydrolysis half-life = NA [8]

Electrochemical data: Meites and Zuman (1977)

Clay-organic interaction data: Davidson et al. (1980), Artiola-Fortung and Fuller (1982).

Solubility: Slightly soluble in water. Soluble in benzene, chloroform, ether, ethanol, carbon tetrachloride. [106],[10],[105],[10],[104],[47],[41]  
 0.45 wt% in water @ 20°C [47],[10]  
 0.46 wt% in water @ 20°C [104]  
 0.45 wt% in water @ 25°C [104]

Form: Colorless to white, off-white, or yellow crystals. Strong, sweet, musky, or medicinal odor. [51],[107],[41]

Use: Organic synthesis; manufacture of industrial and agricultural products; intermediate in the manufacture of the pesticide 2,4-dichlorophenoxyacetic acid (2,4-D) and other compounds for use as germicides, antiseptics, and seed disinfectants; mothproofing; wood preservative. [56],[104],[22],[41]

Fire and explosion hazard: Low.

Flash point: (CC) 113.8°C [107],[51],[22]  
 (OC) 93.3°C [107]

uel: unknown

lel: unknown

Autoign. temp.: unknown

Slightly flammable solid. Slight fire hazard when exposed to heat or flame. When heated to decomposition or on contact with acid or acid fumes, it emits highly toxic fumes of chlorides. Fight fire with CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. Water or foam may cause frothing. [51],[107],[55]

Incompatibility: Acid chlorides; acid anhydrides; oxidizing agents. [51],[55]

## 288 - 2,4-Dichlorophenol

**Handling:** Keep away from heat and flame. Do not breathe vapor or mist (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (butyl rubber gloves, safety goggles, other protective clothing). Use with adequate ventilation (fume hood). Remove contaminated clothing immediately. Safety shower and eye bath stations should be available. Keep container tightly closed. Store in a cool, dry, secure poison area. [56],[57],[55]

**Health effects:** 2,4 DCP is an irritant and potential carcinogen. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include eyes, skin, and respiratory system. It is irritating to mucous membranes and upper respiratory tract. Depending on the intensity and duration of exposure, effects may vary from mild irritation to severe destruction of tissue. Prolonged contact can cause damage to the eyes, severe irritation or burns. May cause second-degree burns after a few minutes of contact. Symptoms of overexposure include tremors, convulsions, shortness of breath, and inhibition of respiratory system. [107],[56],[55]

**Toxicity:** Low

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: 0.21 ppm (1.4 mg/m<sup>3</sup>) [104]

Carcinogenicity: human limited evidence [55]

Mutagenicity: unknown

**Exposure:** Unknown



## 1,2-Dichloropropane



CAS RN: 78-87-5

Syn: 1,2-Dichloropropane \* Propane, 1,2-dichloro- \*  $\alpha,\beta$ -Dichloropropane \* ENT 15406 \* NCI-C55141 \* Propylene chloride \* Propylene dichloride \*  $\alpha,\beta$ -Propylene dichloride \* RCRA Waste Number U083 \*

Molecular formula:  $\text{CH}_3\text{-CHCl-CH}_2\text{Cl}$ 

Polychlorinated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	112.987		
Specific gravity:	1.1558		[10]
	1.15597		[49]
	1.1560		[105]
	1.158		[107]
	1.15597		[15]
Boiling point:	95.0-96°C		[108]
	96.8°C	[51], [104], [47]	
	96.4°C	[10], [107]	
	96.37°C	[49], [105], [16]	
	96.3°C		[22]
	96.1°C		[32]
	96.0°C		[56]
Melting point:	<-70.0°C		[47]
	-80.0°C	[104], [22]	
	-100.0°C	[104], [107], [32]	
	-100.44°C	[10], [49], [105], [16]	
Refractive index:	1.4068		[22]
	1.4388		[108]
	1.4394		[105]
	1.43937	[49], [15]	
	1.4390		[10]
Vapor pressure:	0.133 kPa @ -38.5°C	(1mm) [105], [47]	
	0.667 @ -17.0°C	(5mm) [47]	
	1.333 @ -6.1°C	(10mm) [105], [47]	
	2.67 @ 6.0°C	(20mm) [47]	
	5.333 @ 19.4°C	(40mm) [105], [51]	
	5.27 @ 20°C	(39.5mm) [32]	
	5.60 @ 20°C	(42mm) [104]	
	6.666 @ 25°C	(50mm) [104]	
	6.622 @ 25°C	(49.67mm) [49], [15]	
	8.00 @ 60°C	(60mm) [47]	
	8.800 @ 30°C	(66mm) [104]	
	13.3 @ 39.4°C	(100mm) [105], [47]	
Vapor density:	3.9	[51], [104]	
	3.5		[107]
Evaporation rate:	>1.		[32]
	3.22		[49]
Relative dielectric permittivity:	8.96 @ 25°C		[15]
	8.93 @ 26°C		[11]
	8.925 @ 26.1°C		[49]
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	0.1253 W/(m-K) @ 20°-50°C		[105]
Electrical resistivity:	unknown		

## 290 - 1,2-Dichloropropane

Critical temperature:	304.3°C	[49]
Critical pressure:	4.44 MPa	[49]
Dynamic viscosity:	0.8572 mPa-s @ 20°C	[15], [49]
	0.6739 @ 40°C	[15]
Kinematic viscosity:	0.7415 $\mu\text{m}^2/\text{s}$ @ 20°C	
	0.5830 @ 40°C	
Surface tension:	29. mN/m @ 20°C	[107]
	28.65 @ 20°C	[49], [15]
	27.37 @ 30°C	[49], [15]
	26.15 @ 40°C	[15]
Contact angle:	unknown	
Thermal expansion coefficient:	0.000813 $\text{K}^{-1}$ @ 10°-30°C	[49]
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	6.17 $\times 10^{-30}$ C-m @ 25°C	[49]
	1.46 $\times 10^{-30}$ @ 72°C	[10]
Ionization potential:	10.87 eV (PI)	[105]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	5.83 kJ/mol	[107]
	6.397	[49]
	6.400	[15]
	6.396	[105]
Heat of vaporization:	29.121 kJ/mol	[107]
	31.7778	[10]
	32.004	[49]
	32.026	[15]
	35.2884	[105]
Heat of sublimation:	36.341 kJ/mol	[10]
Heat capacity @ 25°C:	0.09826 kJ/(mol-K) (gas)	[10]
Heat of combustion:	-1883.2 kJ/mol @ 25°C (liq)	[49]
Heat of formation:	-197.9 kJ/mol @ 25°C (liq)	[49]
	-161.96 (gas)	[49]
	-165.80 (gas)	[10]
Gibbs (free) energy:	-83.15 kJ/mol @ 25°C (gas)	[10]
Analytical chemistry: $pP_{\text{oct}}$ =	2.28	[8], [41]
	2.02	[31]
	2.00	[21]
	1.99	[24]
$pK_s$ =	NA	
$pK_a$ =	NA	[31]
$pK_{BH}$ =	NA	
Henry's law constant =	0.23 kPa-m <sup>3</sup> /mol	[41]
	0.210	[24]
	0.298 @ 25°C	[41]
	0.477 @ 37°C	[41]
Hydrolysis half-life =	1.5 $\times 10^7$ to 6.2 $\times 10^7$ sec (est)	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

**Solubility:** Slightly soluble in water. Soluble in ethanol, ether, benzene, chloroform. Miscible with organic solvents.

[105],[108],[10],[104]

0.26 wt% water @ 20°C [32],[22]

0.27 wt% water @ 20°C [104],[10],[47]

0.274 wt% water @ 25°C [49]

0.275 wt% water @ 25°C [14]

**Form:** Colorless, mobile, stable liquid. Sweet, unpleasant, chloroform-like odor. [51],[32],[108],[22]

**Use:** Intermediate for perchloroethylene and carbon tetrachloride; lead scavenger for antiknock fuels; solvent for fats, oils, waxes, gums, resins; soil fumigant for nematodes; in solvent mixtures for cellulose esters and ethers; scouring compound; metal degreasing agent; insecticidal fumigant. [108],[22],[56],[104]

**Fire and explosion hazard:** High.

Flash point: (CC) 15.6°C [107],[32]

(CC) 31°C [49]

(OC) 21°C [108]

(OC) 21.1°C [107]

(OC) 24°C [49]

uel: 14.5% [107],[51],[32],[22],[49]

lel: 3.4% [107],[51],[32],[22],[49]

Autoign. temp.: 557°C [107],[51],[32],[22],[49]

Highly flammable liquid. Can react vigorously with oxidizing materials. Flashback may occur along vapor trail. Toxic gases and vapors (such as carbon monoxide, hydrogen chloride, and phosgene) may be released in a fire. Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder, water. [51],[32],[55]

**Incompatibility:** Oxidizing agents; acids; bases; aluminum and its alloys; o-dichlorobenzene; 1,2-dichloroethane. [51],[55]

**Handling:** Keep away from heat, sparks, and open flame. Avoid prolonged or repeated exposure. Do not inhale vapor or mist (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, on clothing (butyl rubber gloves; protective over-clothing; splash-proof chemical goggles). Remove contaminated clothes immediately. Use with adequate ventilation (fume hood). Keep container tightly closed. Store in a cool, dry, flammable liquid storage area or cabinet. [56],[57],[55]

**Health effects:** 1,2-Dichloropropane is a poison. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include skin, eyes, respiratory system, liver, and kidneys. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Overexposure can cause eye irritation, dermatitis, drowsiness, or light-headedness. Prolonged contact can cause nausea, headache and vomiting. Chronic overexposure may effect the liver and kidneys. It is regarded as one of the more toxic chlorinated hydrocarbons. [51],[32],[56],[55]

**292 - 1,2-Dichloropropane**

**Toxicity: Moderate.**

TWA: 75 ppm (350 mg/m<sup>3</sup>) [1]

STEL: 110 ppm (510 mg/m<sup>3</sup>) [1]

CL: unknown

IDLH: 2000 ppm (9240 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 15-23 ppm (70-106 mg/m<sup>3</sup>) -- not noticeable [32]

50 ppm (235 mg/m<sup>3</sup>) -- recognition [104],[32]

130-190 ppm (600-880 mg/m<sup>3</sup>) -- strong odor [32]

Carcinogenicity: limited animal evidence; possible human [55]

some evidence in small animals [26]

Mutagenicity: unknown

**Exposure: Unknown**

Dieldrin

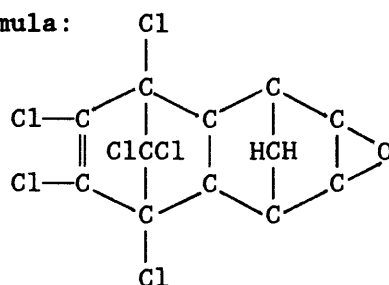
 $C_{12}H_8Cl_6O$ 

CAS RN: 60-57-1

Syn: Dieldrin \* 2,7:3,6-Dimethanonaphth[2,3-*b*]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1a $\alpha$ ,2 $\beta$ ,2a $\alpha$ ,3 $\beta$ ,6 $\beta$ ,6a $\alpha$ ,7 $\beta$ ,7a $\alpha$ )- \* 1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-, *endo,exo*- \* Aldrin epoxide \* Alvit \* Alvit 55 \* Compound 497 \* Dioldrex \* *exo*-Dieldrin \* Dioldrite \* Dioldrix \* Dioldmoth \* Dorytox \* ENT 16225 \* HEOD \* Hexachloroepoxyoctahydro-*endo,exo*-dimethanonaphthalene \* 1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-1,4,5,8-dimethanonaphthalene \* 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-2,7:3,6-dimethanonaphth(2,3-*b*)oxirene \* Illoxol \* Insecticide number 497 \* Insectlack \* Kombi-Albertan \* Moth Snub D \* NA 2761 (DOT) \* NCI-C00124 \* Octalox \* Panoram D-31 \* Quintox \* RCRA Waste Number P037 \* Red Shield \* SD 3417 \* Termitox \*

Structural formula:

Polychlorinated Cyclic Hydrocarbon



Physical properties:

Relative molecular mass:	380.913	
Specific gravity:	1.75	[104], [105], [107]
Boiling point:	decomposes	[107]
Melting point:	175.°C	[22]
	176.°-177°C	[104], [108]
	176.°C	[107]
	175.°-176°C	[105], [56]
	150.°C	[51]
Refractive index:	unknown	
Vapor pressure:	2.37x10 <sup>-8</sup> kPa @ 20°C	(1.78x10 <sup>-7</sup> mm) [56]
	4.1x10 <sup>-7</sup>	@ 20°C (3.1x10 <sup>-6</sup> mm) [108]
	2.4x10 <sup>-8</sup>	@ 25°C (1.8x10 <sup>-7</sup> mm) [104]
Vapor density:	13.2	[104], [51]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	

## 294 - Dieldrin

Electric dipole moment: unknown  
Ionization potential: unknown  
Magnetic volume susceptibility: unknown  
Speed of sound: unknown  
Heat of melting: unknown  
Heat of vaporization: unknown  
Heat of sublimation: unknown  
Heat capacity @ 25°C: unknown  
Heat of combustion: unknown  
Heat of formation: unknown  
Gibbs (free) energy: unknown

Analytical chemistry:  $pP_{oct}$  = 5.16 [27]  
3.54 [31]  
3.692 - 5.16 [41]  
 $pK_s$  = NA  
 $pK_a$  = NA [31]  
 $pK_{BH}$  = NA  
Henry's law constant = 0.00002 kPa·m<sup>3</sup>/mol [41]  
0.0059 [41]  
0.000818 - 0.00322 [41]  
Hydrolysis half-life = >12.5x10<sup>7</sup> sec [8]

Electrochemical data: Unknown

Clay-organic interaction data: Boucher and Lee (1972), Fowker et al. (1960), Huang and Liao (1970).

Solubility: Almost insoluble in water. Slightly soluble in ethanol. Soluble in acetone, benzene, and most common organic solvents except aliphatic petroleum solvents and methyl alcohol. [51],[105],[108],[104],[56]  
0.00001 wt% in water [104]  
0.0000186 wt% in water @ 25°-29°C [56]

Form: White, light brown, or orange-tan crystalline solid. Odorless to mild chemical odor. [51],[55]

Use: Insecticide; stereo isomer of endrin; obtained by oxidation of aldrin; wool processing industry. Primary use in past was control of corn pests, and also used by citrus industry. Dieldrin is extremely apolar, has extremely low volatility and low solubility in water, and therefore persists in the environment with progressive accumulation in the food chain. [56],[104]

Fire and explosion hazard: Very low

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable solid. Emits highly toxic fumes of carbon monoxide, carbon dioxide, and hydrogen chloride gas when heated to decomposition. [51]

Incompatibility: Strong oxidizers; active metals like sodium; strong acids; phenols; copper and its salts; iron and iron salts. [56],[55]

**Handling:** prevent breathing vapors, mist, or dust (appropriate respirator or self-contained breathing apparatus). Prevent any possible skin or eye contact (rubber boots and heavy rubber gloves; safety goggles; protective over-clothing). Employees should wash immediately when skin is wet or contaminated. Work clothing should be changed daily if it is possible that clothing is contaminated. Remove nonimpervious clothing immediately if wet or contaminated. Provide emergency showers and eyewash stations. Use only in well-ventilated area (fume hood). Keep container tightly closed. Store in a cool, dry, secure poison area. [56],[55]

**Health effects:** Dieldrin is an acute toxin and potential carcinogen. Routes of entry are inhalation, skin absorption, ingestion, and eye and skin contact. Points of attack include respiratory system, gastrointestinal system, liver, kidney, skin, and central nervous system. Acts as a central nervous system stimulant and greatly reduces or eliminates appetite. Overexposure can cause: malaise, headache, nausea, vomiting, dizziness, tremors, clonic and tonic convulsions, coma, or respiratory failure. Severe poisoning may result in convulsions, coma, and respiratory failure. [51],[55]

**Toxicity:** Very high.

TWA: 0.016 ppm (0.25 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 29 ppm (450 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 0.041 ppm (0.64 mg/m<sup>3</sup>) [107]

Carcinogenicity: banned by the EPA in October 1974 because of the alleged hazard as a potential carcinogen to humans [107]

indefinite [51]

animal positive [56]

"said to be carcinogenic" [22]

Mutagenicity: neoplastic effects, experimental teratogen, equivalent tumorigenic agent [51]

negative in the *Salmonella* test [104]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: >10 mg/kg body wt -- acute illness [51]

Lethal: 65 mg/kg body wt -- death of an adult [55]

28 mg/kg [55]

Inhalation:

Short-term Inhalation Limits: 0.064 ppm (1 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: unknown

Lethal: unknown

## 296 - Diethyl phthalate

Diethyl phthalate

 $C_{12}H_{14}O_4$ 

CAS RN: 84-66-2

Syn: Diethyl phthalate \* 1,2-Benzenedicarboxylic acid, diethyl ester \*  
 Anozol \* Diethylphthalate \* Diethyl-o-phthalate \* DEP \* Estol 1550 \* Ethyl  
 phthalate \* NCI-C60048 \* Neantine \* Palatinol A \* Phthalic acid, diethyl  
 ester \* Phthalol \* Placidol E \* RCRA Waste Number U088 \* Solvanol \* Unimoll  
 DA \*

Molecular formula: 1,2- $C_6H_4(COOCH_2CH_3)_2$ 

Dicarboxylic Acid Ester

## Physical properties:

Relative molecular mass:	222.241		
Specific gravity:	1.110		[51]
	1.1175		[105], [106]
Boiling point:	302.°C		[51]
	298.°C	[104], [105], [22], [47], [106]	
	295.°C		[10], [108]
Melting point:	-40.5°C	[104], [51], [22]	
	-3.°C		[10], [55]
Refractive index:	1.5000.		[105], [106]
	1.5002		[22]
	1.5049 @ 14°C		[10]
Vapor pressure:	0.0067 kPa @ 70°C	(0.05mm)	[41]
	0.1333 kPa @ 108.8°C	(1mm)	[105]
	1.3332 @ 156°C	(10mm)	[105]
	1.867 @ 163°C	(14mm)	[104]
	4.000 @ 182°C	(30mm)	[104]
Vapor density:	7.66		[104], [51]
Evaporation rate:	unknown		
Relative dielectric permittivity:	unknown		
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	unknown		
Electrical resistivity:	unknown		
Critical temperature:	unknown		
Critical pressure:	unknown		
Dynamic viscosity:	35.0 mPa-s @ 20°C (calc.)		
Kinematic viscosity:	31.3 $\mu m^2/s$ @ 0°C		[22]
Surface tension:	37.5 mN/m @ 20°C		[105], [22]
Contact angle:	unknown		
Thermal expansion coefficient:	unknown		
Compressibility:	unknown		
Vapor diffusivity:	unknown		
Solution diffusivity:	unknown		
Electric dipole moment:	unknown		
Ionization potential:	unknown		
Magnetic volume susceptibility:	-8.11x10 <sup>-6</sup> SI units @ 25°C		[105]
Speed of sound:	unknown		
Heat of melting:	unknown		
Heat of vaporization:	64.406 kJ/mol		[105]
Heat of sublimation:	88.34 kJ/mol		[10]
Heat capacity @ 25°C:	unknown		
Heat of combustion:	unknown		
Heat of formation:	-778.7 kJ/mol @ 25°C		[10]



Gibbs (free) energy: unknown

Analytical chemistry:	pP <sub>oct</sub> =	3.00	[27], [110]
		2.47	[23], [31]
		2.12	[8]
		1.40	[41]
	pK <sub>s</sub> =	NA	
	pK <sub>a</sub> =	NA	[31]
	pK <sub>BB</sub> =	NA	
	Henry's law constant =	0.000086 kPa·m <sup>3</sup> /mol	[41]
	Hydrolysis half-life =	5.8x10 <sup>8</sup> sec	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Soluble in acetone, benzene. Miscible with ethanol, ether, esters, ketones. [105], [104], [41]

0.0210 wt% in water	[104]
0.0896 wt% in water @ 25°C	[41]
0.108 wt% in water @ 25°C	[23]

Form: Paper-white to colorless liquid. Odorless to mild chemical odor. [51], [56], [41]

Use: Solvent for cellulose esters; vehicle in pesticide sprays; fixative and solvent in perfumery; alcohol denaturant; plasticizer in solid rocket propellants; plastics manufacture and processing; suitable for food packaging application (FDA); dye application agent; diluent in polysulfide dental impression materials solvent; wetting agent; camphor substitute; component in insecticidal sprays; mosquito repellent. [56], [104]

Fire and explosion hazard: Low.

Flash point: (OC) 163°C [51], [22]

Uel: unknown

lel: 0.75% @ 187°C [55]

Autoign. temp.: 457°C [55]

Combustible liquid. Emits acrid smoke and CO and CO<sub>2</sub> when heated to decomposition. Fight fire with water, dry chemical powder, alcohol or polymer foam. Foam and water spray are effective but may cause frothing. [51], [22], [55]

Incompatibility: Oxidizing agents; acids. [55]

Handling: Avoid heat, flame, and sources of ignition. Prevent inhalation of vapor or mist (appropriate respirator or self-contained breathing apparatus). Avoid prolonged or repeated exposure. Do not get in eyes, on skin, on clothing (protective overclothing; splash-proof chemical goggles; rubber gloves). Keep container tightly closed. Store in a cool, dry place. [56], [55]

## 298 - Diethyl phthalate

**Health effects:** DEP can be a mild irritant. Routes of entry are ingestion, inhalation, skin absorption, and eye and skin contact. Points of attack include eyes, skin, respiratory system. Heated vapor or mist can be irritating to the eyes, mucous membranes and upper respiratory tract. Has few acute or chronic toxic properties and seems to be devoid of any major irritating or sensitizing effects on the skin. Other sited symptoms are conjunctivitis, corneal necrosis, respiratory tract irritation, eczema, nausea, dizziness, and headache. Chronic exposure may cause reproductive disorder(s) based on tests with laboratory animals. [56],[55]

### **Toxicity: Low**

TWA: 0.55 ppm (5 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: odorless [51]

Carcinogenicity: no evidence [56]

Mutagenicity: experimental teratogen [51],[55]

### **Exposure:**

#### **External:**

Non-lethal: unknown

Lethal: unknown

#### **Oral:**

Non-lethal: unknown

Lethal: unknown

#### **Inhalation:**

Short-term Inhalation Limits: unknown

Non-lethal: 110 ppm (1000 mg/m<sup>3</sup>) -- systemic irritant effects [51]

Lethal: unknown

Dimethyl phthalate

 $C_{10}H_{10}O_4$ 

CAS RN: 131-11-3

Syn: Dimethyl phthalate \* 1,2-Benzenedicarboxylic acid, dimethyl ester \* Avolin \* Dimethyl-1,2-benzenedicarboxylate \* Dimethyl benzeneorthodicarboxylate \* Dimethyl ester 1,2-benzenedicarboxylic acid \* o-Dimethylphthalate \* Dimethyl-o-phthalate \* DMP \* ENT 262 \* Fermine \* Methyl phthalate \* Mipax \* NTM \* Palatinol M \* Phthalic acid, dimethyl ester \* Phthalic acid, methyl ester \* RCRA Waste Number U102 \* Repeftal \* Solvanom \* Solvarone \* Unimoll DM \*

Molecular formula: 1,2- $C_6H_4(COOCH_3)_2$ 

Dicarboxylic Acid Ester

**Physical properties:**

Relative molecular mass:	194.187		
Specific gravity:	1.189 @ 25/25		[51], [22]
	1.19 @ 25/25		[104]
	1.1905		[105]
	1.940 @ 20/20		[10]
	1.2		[32]
Boiling point:	285.0°C		[56], [32]
	283.8°C		[105]
	283.7°C		[10], [51]
	282.0°C		[22]
Melting point:	0-2.0°C		[105], [32]
	5.5°C		[10], [23]
Refractive index:	1.515 @ 21°C		[10]
	1.5138 @ 20°C		[105]
Vapor pressure:	<0.0013 @ 20°C	(<0.01mm)	[104]
	0.133 @ 100.3°C	(1mm)	[51], [32]
	0.133 kPa @ 100°C	(1mm)	[104]
	1.333 @ 147.6°C	(10mm)	[105]
	5.333 @ 182.8°C	(40mm)	[105]
Vapor density:	6.69		[51]
	6.7 @ BP		[32]
Evaporation rate:	≈0.		[32]
Relative dielectric permittivity:	8.5 @ 24°C		[105], [10]
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	unknown		
Electrical resistivity:	unknown		
Critical temperature:	unknown		
Critical pressure:	unknown		
Dynamic viscosity:	17.2 mPa-s @ 25°C		[108]
	9.18 @ 35°C		[10]
Kinematic viscosity:	14.5 $\mu m^2/s$ @ 25°C		
	7.71 @ 35°C		
Surface tension:	unknown		
Contact angle:	unknown		
Thermal expansion coefficient:	unknown		
Compressibility:	unknown		
Vapor diffusivity:	unknown		
Solution diffusivity:	unknown		
Electric dipole moment:	unknown		
Ionization potential:	9.75 eV		[41]

### 300 - Dimethyl phthalate

Magnetic volume susceptibility: unknown  
Speed of sound: unknown  
Heat of melting: unknown  
Heat of vaporization: 62.48 kJ/mol [105]  
Heat of sublimation: unknown  
Heat capacity @ 25°C: unknown  
Heat of combustion: 4687.96 kJ/mol @ 20°C [105]  
4690.3 kJ/mol [22]  
Heat of formation: -678.3 kJ/mol @ 25°C [10]  
Gibbs (free) energy: unknown

Analytical chemistry:  $pP_{oct}$  = 2.12 [8]  
2.00 [27]  
1.56 [31]  
1.47 - 2.00 [41]  
 $pK_s$  = NA  
 $pK_a$  = NA [31]  
 $pK_{BH}$  = NA  
Henry's law constant = 0.000043 kPa-m<sup>3</sup>/mol [41]  
Hydrolysis half-life = 1.01x10<sup>8</sup> sec [8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water and petroleum ether. Miscible with benzene, ethanol, ether and chloroform. [105],[108]

0.5 wt% in water @ 20°C [104]  
0.04 wt% in water @ 20°C [32]  
0.4 wt% in water @ 25°C [23]  
0.43 wt% in water [10]

Form: Colorless, odorless, oily liquid. Pale yellow crystals. [51],[56]

Use: As a plasticizer for nitrocellulose, cellulose ester plastics, cellulose acetate, resins, rubber, elastomers, solid rocket propellants; in lacquers, plastics, rubber, coating agents, safety glass, molding powders, perfumes, insect repellent. [56],[104],[22],[41]

Fire and explosion hazard: Low.

Flash point: (CC) 146.°C [51],[32]

uel: 8.03% @ 229°C [55]

lel: 1.2% @ 146°C [32]

0.94% @ 181°C [55]

Autoign. temp.: 555.6°C [51],[22],[32]

Slightly flammable liquid. May react with oxidizing materials. When heated to decomposition it emits acrid smoke and fumes, including CO and CO<sub>2</sub>. Fight fire with water spray, dry chemical powder, alcohol or polymer foam, CO<sub>2</sub>. Foam and water spray are effective but may cause frothing. [51],[32],[55]

Incompatibility: Nitrates; strong oxidizers; strong alkalies; strong acids. [56],[55]

**Handling:** Keep away from heat and open flame. Do not breathe vapor (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (chemical resistant gloves, safety goggles, other protective clothing). Use with good ventilation (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [57],[55]

**Health effects:** DMP is an irritant. Routes of entry are ingestion, inhalation, and eye and skin contact. Points of attack include respiratory system, eyes, gastrointestinal system. Vapor or mist is irritating to the eyes, skin, mucous membranes and upper respiratory tract. Exposure can cause nausea, dizziness and headache. Chronic overexposure may cause reproductive disorders. [56],[55]

**Toxicity:** Low

TWA: 0.63 ppm (5 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: 1170 ppm (9300 mg/m<sup>3</sup>) [56]

Peak: unknown

Odor threshold: unknown

Carcinogenicity: unknown

Mutagenicity: experimental teratogen [51],[55]

**Exposure:** Unknown

## 302 - Dimethyl sulfoxide

Dimethyl sulfoxide

 $C_2H_6OS$ 

CAS RN: 67-68-5

Syn: Dimethyl sulfoxide \* Methane, sulfinylbis- \* A 10846 \* Deltan \*  
 Demasorb \* Demavet \* Demeso \* Demsodrox \* Dermasorb \* Dimethyl sulphoxide \*  
 Dimexide \* Dipirartril-tropico \* DMS-70 \* DMS-90 \* DMSO \* Dolicur \* Doligur  
 \* Domoso \* Domosol \* Dromisol \* Durasorb \* Gamasol 90 \* Hyadur \* Infiltrina  
 \* M-176 \* Methylsulfinylmethane \* Methyl sulfoxide \* Methylthiomethane \*  
 NSC-763 \* Rimso-50 \* Somipront \* SQ 9453 \* Sulfinylbis[methane] \* Syntexan  
 \* Topsym (rescinded) \*

Molecular formula:  $CH_3SOCH_3$ 

Oxo-sulphur Hydrocarbon

## Physical properties:

Relative molecular mass:	78.12904	
Specific gravity:	1.10041	[49]
	1.100	[10], [51]
	1.01	[22]
	1.1014	[105], [106]
Boiling point:	189.0°C	[10], [49], [51], [22], [105]
Melting point:	18.54°C	[49]
	18.5°C	[10], [51], [22]
	18.4°C	[105], [106]
Refractive index:	1.47933	[49]
	1.4783	[10]
	1.4770	[105]
	1.4170	[106]
Vapor pressure:	0.0493 kPa @ 20°C (0.370mm)	[51]
Vapor density:	2.7	[55]
Evaporation rate:	unknown	
Relative dielectric permittivity:	48.9 @ 20°C	[22]
	46.45 @ 25°C	[49]
	46.6 @ 25°C	[10]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	5. MOhm-m @ 25°C	[49]
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	2.2159 mPa-s @ 20°C	[49]
	1.991 @ 25°C	[49]
	1.996 @ 25°C	[10]
	1.654 @ 30°C	[49]
Kinematic viscosity:	2.0137 $\mu m^2/s$ @ 20°C	
	1.809 @ 25°C	
	1.815 @ 25°C	
	1.503 @ 30°C	
Surface tension:	43.54 mN/m @ 25°C	[10]
Contact angle:	unknown	
Thermal expansion coefficient:	0.000928 K <sup>-1</sup>	[49]
Compressibility:	0.52 nPa <sup>-1</sup> @ 25°C	[49]
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	

Electric dipole moment:	13.54x10 <sup>-30</sup> C-m	[49]
	13.21x10 <sup>-30</sup>	[105]
	13.01x10 <sup>-30</sup>	[10]
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	14.368 kJ/mol	[49]
	6.531	[10]
Heat of vaporization:	43.14 kJ/mol	[49]
	53.00	[10]
Heat of sublimation:	77.0 kJ/mol	[49]
	52.92	[10]
Heat capacity @ 25°C:	0.15318 kJ/(mol-K) (liq)	[49]
	0.1474 (liq)	[10], [105]
	0.0890 (gas)	[105]
	0.2290	[22]
Heat of combustion:	-1979. kJ/mol @ 25°C (liq)	[107]
Heat of formation:	-203.89 kJ/mol @ 25°C (liq)	[49]
	-203.48 @ 25°C (liq)	[10], [105]
	-151.01 (gas)	[49]
	-150.56 (gas)	[105]
Gibbs (free) energy:	-99.23 kJ/mol @ 25°C (liq)	[10], [105]
	-81.56 (gas)	[105]
Analytical chemistry:	pP <sub>oct</sub> = -1.35	[21]
	pK <sub>s</sub> = 31.8 @ 25°C	[49]
	17.3 @ 25°C	[10]
	pK <sub>a</sub> = 1.4 in acetic acid anhydride	[49]
	-1.54 @ 25°C in aq H <sub>2</sub> SO <sub>4</sub>	[49]
	pK <sub>BH</sub> = unknown	
	Henry's law constant = unknown	
	Hydrolysis half-life = unknown	

Electrochemical data: Meites and Zuman (1977)

Clay-organic interaction data: Jacobs and Sterckx (1970), Andrews et al. (1967)

Solubility: Soluble in water, ethanol, ether, acetone, benzene, chloroform. Dissolves some hydrocarbons more than others. Extremely powerful aprotic solvent; hygroscopic liquid. [10],[22],[49]  
25.3 wt% in water @ 25°C [49]

Form: Colorless, liquid. Practically odorless to that of decayed vegetables. Slightly bitter taste with sweet after-taste. [51],[107]

Use: Solvent for polymerization and cyanide reactions, acetylene, sulfur dioxide and other gases; analytical reagent; solvent for Orlon; spinning polyacrylonitrile and other synthetic fibers; industrial cleaners, pesticides, paint stripping; hydraulic fluids; preservation of cells at low temperatures; diffusion of drugs, etc., into blood stream by topical application; medicine; plant pathology and nutrition; pharmaceutical products; as paint and varnish remover. [22],[104],[56]

### 304 - Dimethyl sulfoxide

**Fire and explosion hazard:** Low.

Flash point: (CC) 87.8°C [107]  
(OC) 95°C [51],[22]

uel: 28.5% [51]

lel: 2.6% [51]

Autoign. temp.: 215°C [51]

Combustible liquid. Low fire hazard when exposed to heat or flame. When heated to decomposition it emits toxic fumes (sulfur dioxide, formaldehyde, methyl mercaptan, carbon monoxide, carbon dioxide). Can react violently with oxidizing materials. Fight fire with water, alcohol or polymer foam, dry chemical powder, CO<sub>2</sub>. [51],[107],[22],[55]

**Incompatibility:** Strong oxidizing agents; strong acids; strong reducing agents; acyl and aryl halides; boron compounds; N<sub>2</sub>O<sub>4</sub>; IF<sub>2</sub>; metal oxosalts; non-metal halides; silver difluoride; many acyl and aryl halides; bromobenzyl acetanilide; sulfur trioxide; acid chlorides; phosphorus halides. Methyl sulfoxide undergoes a violent exothermic reaction on mixing with copper wool and trichloroacetic acid. On mixing with potassium permanganate, it will flash instantaneously. It reacts violently with: acid halides, cyanuric chloride, silicon tetrachloride, phosphorus trichloride and trioxide, thionyl chloride, magnesium perchlorate, silver fluoride, methyl bromide, iodine pentafluoride, nitrogen periodate, diborane, sodium hydride, perchloric and periodic acids. [51],[56],[55]

**Handling:** Avoid heat or flame. Avoid breathing vapors, airborne spray, or droplets (appropriate respirator or self-contained breathing apparatus). Avoid skin or eye contact (neoprene, natural rubber or latex gloves; chemical safety goggles; lab coat). Wash contaminated clothing before reuse. Safety shower and eye bath stations should be available. Use with adequate ventilation (fume hood). Keep container tightly closed. Store in a cool dry place. [56],[57],[55]

**Health effects:** DMSO is an irritant. Routes of entry are ingestion, inhalation, absorption through skin, and eye and skin contact. Points of attack include upper respiratory system, skin, and eyes. Systemic reactions include nausea, vomiting, chills, cramps and lethargy. It freely penetrates the skin. Overexposure may result in skin irritation with redness, burning, itching and sometimes scaling. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. It may cause allergic respiratory and skin reactions. [51],[56],[55]

**Toxicity:** Low.

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: 0.0003-0.016 ppm (0.001-0.05 mg/m<sup>3</sup>) [104]  
practically no odor [107]

Carcinogenicity: none [104]

Mutagenicity: experimental teratogen [51].  
none in the *Salmonella* test [104]



**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: >15 g/kg body wt -- 50% chance of death [107]

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown

### 306 - 2,4-Dinitrophenol

2,4-Dinitrophenol

$C_6H_4N_2O_5$

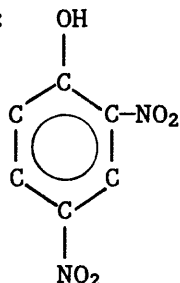
CAS RN: 51-28-5

Syn: 2,4-Dinitrophenol \* Phenol, 2,4-dinitro- \* Aldifen \* Chemox PE \*  $\alpha$ -Dinitrophenol \* DNP \* 2,4-DNP \* Fenoxyl carbon n \* 1-Hydroxy-2,4-dinitrobenzene \* Maroxol-50 \* Nitro kleenup \* Nitrophen \* Nitrophenene \* NSC 1532 \* Phenol,  $\alpha$ -Dinitro- \* RCRA Waste Number P048 \* Solfo black B \* Solfo black BB \* Solfo black 2B supra \* Solfo black G \* Solfo black SB \* Tertrosulphur black PB \* Tertrosulphur PBR \*

Molecular formula:  $HO-C_6H_3-(NO_2)_2-2,4$

Nitrobenzene

Structural formula:



#### Physical properties:

Relative molecular mass:	184.108	
Specific gravity:	1.683 @ 24°C	[104], [10], [51], [105]
	1.68 @ 20°C	[107], [55]
Boiling point:	sublimes at melting pt	[10], [105]
Melting point:	112.°C	[51]
	112.°-114°C	[10]
	113.°C	[107]
	115.°-116°C	[105]
	111.°-114°C	[104], [108]
Refractive index:	unknown	
Vapor pressure:	1.99x10 <sup>-6</sup> kPa @ 18°C (1.49x10 <sup>-5</sup> mm)	[41]
	5.2x10 <sup>-5</sup> @ 20°C (3.9x10 <sup>-4</sup> mm)	[41]
	>0.	[23]
Vapor density:	6.35	[51], [55]
	6.36	[104]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	



### 308 - 2,4-Dinitrophenol

Combustible solid. Explosive powder. May detonate when heated under confinement. When heated to decomposition emits toxic fumes of carbon monoxide, carbon dioxide, and nitrogen oxides. Fight fire with water, alcohol or polymer foam, dry chemical powder, or CO<sub>2</sub>. [51],[107],[55]

**Incompatibility:** Oxidizing materials and combustibles; heavy metals and their compounds. [56]

**Handling:** Keep away from heat, sparks, and open flame. May be shock-sensitive. It may be shock-sensitive. Prevent contact with skin and eyes (laboratory coat, safety goggles or face mask; butyl rubber gloves, boots). Use appropriate respirator or self-contained breathing apparatus to prevent inhalation. Use only in a well-ventilated area (fume hood). Keep container tightly closed. Store in a cool, dry, well-ventilated secure poison area. [56],[107],[55]

**Health effects:** DNP is a poison. Routes of entry are percutaneous absorption, inhalation, and ingestion. Points of attack include skin, liver, eyes, and central nervous system. Symptoms include headache, loss of appetite, vomiting, abdominal pain, diarrhea, fever, chest pains, dizziness, fatigue, jaundice, leg cramps, cyanosis, anxiety, pulmonary edema, and convulsions. This substance produces a marked increase in metabolism and temperature, profuse sweating, nausea, vomiting, collapse, and death. Prolonged exposure can cause dermatitis, cataracts, weight loss, granulocytopenia, polyneuropathy, liver damage, or exfoliative dermatitis. [108],[107],[56],[55]

**Toxicity:** Moderate.

TWA: no values set [1]

STEL: no values set [1]

CL: unknown

IDLH: 0.66 ppm (5.0 mg/m<sup>3</sup>) [107]

Peak: unknown

Odor threshold: unknown

Carcinogenicity: unknown

Mutagenicity: probable [51]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: 1-3 g in adults [108]

4.3 mg/kg body wt -- death of an adult human [51]

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: >0.13 ppm (1 mg/m<sup>3</sup>) -- unsatisfactory [104]

Lethal: unknown

2,4-Dinitrotoluene

 $C_7H_5N_2O_4$ 

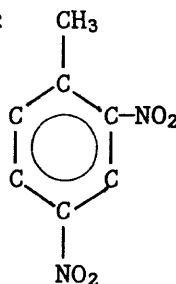
CAS RN: 121-14-2

Syn: 2,4-Dinitrotoluene \* Benzene, 1-methyl-2,4-dinitro- \* 2,4-Dinitrotoluol \* DNT \* 2,4-DNT \* 1-Methyl-2,4-dinitrobenzene \* NCI-C01865 \* RCRA Waste Number U105 \* Toluene, 2,4-dinitro- \*

Molecular formula:  $(NO_2)_2C_6H_3 \cdot CH_3$ 

Nitrobenzene

Structural formula:



## Physical properties:

Relative molecular mass:	182.136	
Specific gravity:	1.321 @ 71°C	[47], [10]
	1.32 (liq)	[32]
	1.3208 @ 71°C	[22], [105]
	1.379	[107]
	1.52 (sol)	[32]
	1.521 @ 15°C	[104], [51]
Boiling point:	250.°C (slow decomp.)	[32]
	270.°C (self-sustained decomp.)	[32]
	300.°C (slight decomp.)	[51], [105], [10], [104]
Melting point:	64.°-66°C	[10]
	69.5°C	[51]
	70.°C	[32], [47], [107], [104]
	70.5°C	[22]
	71.°C	[105], [106], [56]
		[10], [105], [106]
Refractive index:	1.442	
Vapor pressure:	0.00068 kPa @ 20°C	(0.0051mm) [41]
	0.0000147 @ 20°C	(0.00011mm) [41]
	0.133 @ 20°C	(1mm) [32]
	0.000173 @ 58.8°C	(0.0013mm) [41]
	0.00052 @ 69.1°C	(0.0039mm) [41]
	0.133 @ 102.7°C	(1mm) [55]
Vapor density:	6.27	[51], [104]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	

### 310 - 2,4-Dinitrotoluene

Compressibility: NA  
Vapor diffusivity: unknown  
Solution diffusivity: unknown  
Electric dipole moment: unknown  
Ionization potential: unknown  
Magnetic volume susceptibility: unknown  
Speed of sound: unknown  
Heat of melting: 20.13 kJ/mol [107]  
20.12 [105]  
Heat of vaporization: 70.92 kJ/mol [107]  
Heat of sublimation: unknown  
Heat capacity @ 25°C: unknown  
Heat of combustion: -3518. kJ/mol @ 25°C (sol) [107]  
Heat of formation: -71.6 kJ/mol @ 25°C (sol) [10]  
Gibbs (free) energy: unknown

Analytical chemistry:  $pP_{oct}$  = 2.01 [8]  
1.98 [21], [31], [41]  
 $pK_s$  = NA  
 $pK_a$  = NA [31]  
 $pK_{BH}$  = NA  
Henry's law constant = 0.000088 kPa-m<sup>3</sup>/mol [41]  
Hydrolysis half-life = NA [8]

Electrochemical data: Meites and Zuman (1977)

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water. Soluble in alcohol, ethanol, acetone, benzene, pyrimidine, carbon disulfide. [57], [45], [23], [56], [10]  
0.03 wt% in water @ 20°C [23]  
0.0270 wt% in water @ 22°C [56]  
0.03 wt% in water @ 22°C [45], [10], [22]  
1.2 wt% in alcohol @ 15°C [45], [10]  
9. wt% in ether @ 15°C [45], [10]

Form: Red or orange to yellow needles (solid) or yellow liquid.  
Characteristic weak odor. [49], [23], [41]

Use: Organic synthesis; intermediate for toluidines, dyes, explosives.  
[20], [41]

Fire and Explosion Hazard: Low.

Flash point: (CC) 206.7°C [105]  
(OC) 206.7°C [49], [23]

uel: unknown

lel: unknown

Autoign. temp.: unknown

Very slightly flammable solid. Moderate explosion hazard when in the form of dust. When heated to decomposition it emits toxic fumes of nitrogen oxides, CO, and CO<sub>2</sub>. Material may be shock-sensitive. To fight fire use water spray, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam.  
[49], [23], [53]

**Incompatibility:** Strong oxidizers; nitric acid; reducing agents; strong bases; chemically active metals such as tin and zinc. It is stable at temperatures below 250°C. [49],[23],[53]

**Handling:** Any possible contact with this substance should be avoided. Keep away from heat and open flame. Do not breathe dust, mist or vapor (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, on clothing (heavy rubber gloves; safety goggles; other protective clothing). Readily absorbed through skin. Use in well-ventilated area (fume hood). Provide safety showers and eye bath stations. Keep container tightly closed. Store in a cool, dry, secure poison area. [105],[53]

**Health Effects:** 2,4-DNT is a poison. Routes of entry are inhalation of vapor, percutaneous absorption of liquid, and eye and skin contact. Points of attack include blood, liver, cardiovascular system. It is readily absorbed through the skin. Even a small amount absorbed from clothes or shoes may cause toxic symptoms. Short-term exposure may cause a bluish discoloration of the skin, headache, irritability, dizziness, weakness, nausea, vomiting, shortness of breath, drowsiness, and unconsciousness. If treatment is not given promptly, death may occur. Repeated or prolonged exposure can cause anemia, methemoglobinemia leading to anoxia, cyanosis and liver damage. Onset of symptoms may be delayed 2 to 4 hours or longer. Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. [23],[49],[54],[53]

**Toxicity: High**

TWA: 0.20 ppm (1.5 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 26.8 ppm (200 mg/m<sup>3</sup>) [105],[54]

Peak: unknown

Odor threshold: unknown

Carcinogenicity: positive rat, negative mouse [49],[105]

Mutagenicity: experimental neoplastic effects [49]

**Exposure: Unknown**

## 312 - 2,6-Dinitrotoluene

2,6-Dinitrotoluene

 $C_7H_6N_2O_4$ 

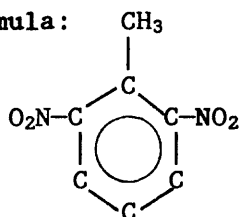
CAS RN: 606-20-2

Syn: 2,6-Dinitrotoluene \* Benzene, 2-methyl-1,3-dinitro- \* 2,6-DNT \* 2-methyl-1,3-dinitrobenzene \* RCRA Waste Number U106 \*

Molecular formula:  $CH_3-C_6H_3-(NO_2)_2$ 

Aromatic Nitro-Hydrocarbon

Structural formula:



## Physical properties:

Relative molecular mass:	182.136	
Specific gravity:	1.289 @ 111°C	[10]
	1.2833 @ 111°C	[10], [105]
	1.283 @ 111°C	[107]
Boiling point:	Decomposes	[107]
	285°C	[23]
Melting point:	64.°-66°C	[10], [104]
	66°C	[105]
	60.5°C	[107]
Refractive index:	1.479	[10], [105]
Vapor pressure:	0.47x10 <sup>-4</sup> kPa @ 20°C (3.5x10 <sup>-4</sup> mm)	[23]
	0.002 @ 20°C (0.018mm)	[31]
Vapor density:	6.28	[107]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	unknown	
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	unknown	
Heat of combustion:	-3429.6 kJ/mol @ 25°C (sol)	[105]
Heat of formation:	-51.08 kJ/mol @ 25°C (sol)	[10]



Gibbs (free) energy: unknown

Analytical chemistry:	$pP_{oct} =$	2.28	[31]
		2.05	[8]
		2.00	[41]
		1.72	[23]
	$pK_s =$	NA	
	$pK_a =$	NA	[31]
	$pK_{BH} =$	NA	
	Henry's law constant =	0.0000220 kPa·m <sup>3</sup> /mol	[41]
	Hydrolysis half-life =	NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water. Soluble in ethanol. [10],[105],[41]  
0.03 wt% in water [41]

Form: Orange-yellow or tan crystals. [107],[55]

Use: Manufacture of TNT, urethane polymers, flexible and rigid foams and surface coatings, and dyes; organic synthesis. [56],[104]

Fire and explosion hazard: Low.

Flash point: (CC) 404°C (est) [107]  
(??) 206.7°C (calc) [41]

uel: unknown

lel: unknown

Autoign. temp.: unknown

Slightly flammable solid. Dust may explode when exposed to heat or flame. It is a combustible substance and produces toxic NO<sub>x</sub> fumes when it burns. Fight fire with water spray, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [107],[51],[55]

Incompatibility: Strong oxidizers; caustics; metals such as tin and zinc; reducing agents; strong bases. [56],[55]

Handling: Avoid all contact. Keep away from heat and flame. Do not breathe dust or fumes (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, on clothing (rubber boots and heavy rubber gloves; chemical safety goggles; other protective overclothing). Wash immediately when skin is wet or contaminated and daily at the end of each work shift. Work clothing should be changed daily if it is possible that the clothing is contaminated. Remove nonimpervious clothing immediately if wet or contaminated. Provide emergency showers and eye bath stations. Keep container tightly closed. Store in a cool, dry, secure poison area. [107],[56],[55]

### 314 - 2,6-Dinitrotoluene

**Health effects:** 2,6-DNT is highly toxic. Routes of entry are inhalation of vapor, percutaneous absorption of liquid, ingestion, and eye and skin contact. Points of attack include the blood, liver, and cardiovascular system. No local effects. Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis and anoxia. Onset may be delayed 2 to 4 hours or longer. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, irritability, weakness, headache, nausea and vomiting, dyspnea, drowsiness, and unconsciousness. If treatment is not given promptly, death may occur. Repeated or prolonged exposure may cause anemia. Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. [56],[22],[55]

**Toxicity:** High.

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: 27 ppm (200 mg/m<sup>3</sup>) [107]

Peak: unknown

Odor threshold: 0.1 ppm (0.75 mg/m<sup>3</sup>) in water [104]

Carcinogenicity: unknown

Mutagenicity: unknown

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: 50-500 mg/kg body wt -- 50% chance of death [107]

Inhalation:

Short-term Inhalation Limits: 0.65 ppm (5 mg/m<sup>3</sup>) [107]

Non-lethal: unknown

Lethal: unknown

1,4-Dioxane

 $C_4H_8O_2$ 

CAS RN: 123-91-1

Syn: 1,4-Dioxane \* Diethylene dioxide \* 1,4-Diethylene dioxide \* Diethylene ether \* Diethylene oxide \* Di(ethylene oxide) \* Diokan \* 1,4-Dioxacyclohexane \* Dioxan \* Dioxane \* Dioxane-1,4 \* *p*-Dioxane \* *p*-Dioxin, tetrahydro- \* Dioxyethylene ether \* Glycol ethylene ether \* NCI-C03689 \* RCRA Waste Number U108 \* Tetrahydro-*p*-dioxin \* Tetrahydro-1,4-dioxin \* UN 1165 (DOT) \*

Molecular formula:  $OCH_2CH_2OCH_2CH_2$ 

Aliphatic Cyclic Ether

**Physical properties:**

Relative molecular mass:	88.1063	
Specific gravity:	1.036	[107]
	1.0353	[51]
	1.0337	[105], [106]
	1.03361	[49]
	1.033	[104], [47]
	1.0329	[10], [108]
Boiling point:	1.03	[32]
	101.°C	[32], [104], [105]
	101.1°C	[51], [108], [47]
	101.2°C	[10]
	101.3°C	[22], [107]
	101.320°C	[49]
Melting point:	12.°C	[51]
	11.80°C	[108], [105], [32], [49], [107]
	11.7°C	[10]
	10.°-12°C	[22]
	9.5°-10.5°C	[47]
Refractive index:	1.4221	[22]
	1.4224	[10], [105], [106]
	1.42241	[49]
Vapor pressure:	0.133 kPa @ -35.8°C	(1mm) [47]
	0.667 @ -12.8°C	(5mm) [47]
	1.33 @ -1.2°C	(10mm) [47]
	2.67 @ 12.0	(20mm) [47]
	3.87 @ 20°C	(29mm) [32]
	4.00 @ 20°C	(30mm) [104]
	4.95 @ 25°C	(37.1mm) [104], [49]
	5.33 @ 25.2°C	(40mm) [51], [47]
	6.135 @ 30°C	(46.02mm) [49]
	6.67 @ 30°C	(50mm) [104]
	8.00 @ 33.8°C	(60mm) [47]
	13.3 @ 45.1°C	(100mm) [47]
Vapor density:	3.0	[32]
	3.03	[104], [51]
Evaporation rate:	2.42	[49]
	2.7	[32]

## 316 - 1,4-Dioxane

Relative dielectric permittivity:	2.224 @ 15°C	[2]
	2.220 @ 20°C	[2]
	2.205 @ 25°C	[2]
	2.209 @ 25°C	[105], [10], [49]
	2.21 @ 25°C	[11]
	2.200 @ 30°C	[2]
	2.153 @ 50°C	[2]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	$2. \times 10^6$ MOhm-m @ 25°C	[49], [11]
Critical temperature:	311.8°C	[20]
	312.°C	[108]
	314.°C	[10], [49], [107]
	314.8°C	[105]
Critical pressure:	5.14 MPa	[108], [20]
	5.21	[105], [10], [49], [107]
Dynamic viscosity:	1.439 mPa-s @ 15°C	[10], [49]
	1.20 @ 25°C	[108]
	1.087 @ 30°C	[49]
Kinematic viscosity:	1.397 $\mu\text{m}^2/\text{s}$ @ 15°C	
	1.17 @ 25°C	
	1.052 @ 30°C	
Surface tension:	36.23 mN/m @ 0°C	[10]
([10] values are calculated)	34.84 @ 10°C	[10]
	34.45 @ 15°C	[49]
	33.75 @ 20°C	[49]
	33.45 @ 20°C	[10]
	32.80 @ 25°C	[49]
	32.06 @ 30°C	[10]
Contact angle:	unknown	
Thermal expansion coefficient:	0.001115 K <sup>-1</sup>	[49]
Compressibility:	$7.38 \times 10^{-7}$ nPa <sup>-1</sup> @ 25°C	[49]
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	0. C-m	[108], [10]
	$1.50 \times 10^{-30}$	[49]
Ionization potential:	9.13 eV (PI)	[105]
Magnetic volume susceptibility:	$-7.6 \times 10^{-6}$ SI units @ 32°C	[105]
Speed of sound:	unknown	
Heat of melting:	12.460 kJ/mol	[49]
	12.48	[108]
	12.847	[105]
	12.85	[10]
	12.86	[107]
Heat of vaporization:	35.585 kJ/mol	[49]
	35.78	[105]
	36.4	[107]
Heat of sublimation:	38.52 kJ/mol	[10]
Heat capacity @ 25°C:	0.15065 kJ/(mol-K) (liq)	[49]
	0.1507 (liq)	[105]
	0.09411 (gas)	[10]
Heat of combustion:	-2363.92 kJ/mol @ 25°C (liq)	[108]

Heat of formation:	-353.55 kJ/mol @ 25°C (liq)	[49]
	-353.7 (liq)	[10]
	-315.2 (gas)	[10]
Gibbs (free) energy:	-188.2 kJ/mol @ 25°C (liq)	[10]
	-180.9 (gas)	[10]
Analytical chemistry: $pP_{oct}$ =	-0.42	[104],[21]
	-0.27	[21],[24]
	$pK_s$ = unknown	
	$pK_a$ = -1.83 @ 25°C	[49]
	$pK_{BH}$ = unknown	
	Henry's law constant = 0.000495 kPa·m <sup>3</sup> /mol	[24]
	Hydrolysis half-life = unknown	

**Electrochemical data:** Unknown

**Clay-organic interaction data:** Brindley et al. (1969), Brindley and Tsunashima (1972), Laby (1962), Hoffmann and Brindley (1962), Carr and Chih (1971)

**Solubility:** Miscible with water, ethanol, ether, acetone, benzene, acetic acid, and other organic solvents. [49],[108],[105],[32].

**Form:** Colorless, volatile, liquid with a faint, pleasant, somewhat alcoholic, ethereal odor. Hygroscopic and will produce peroxides in the presence of moisture. [51],[32],[107],[56]

**Use:** Solvent for cellulose acetate, ethyl cellulose, benzyl cellulose, resins, oils, waxes, oil and spirit-soluble dyes, and many other organic as well as some inorganic compounds; lacquers; paints; varnishes; paint and varnish removers; wetting and dispersing agent in textile processing; dye baths; stain and printing compositions; cleaning and detergent preparations; cements; cosmetics; deodorants; fumigants; emulsions; polishing compositions; stabilizer for chlorinated solvents; in scintillation counters. [22],[108],[104],[56]

**Fire and explosion hazard:** High

Flash point: (CC) 18°C [108],[22]  
 (CC) 12.2°C [51],[107]  
 (CC) 12°C [49]  
 (OC) 23°C [49]  
 (OC) 23.3°C [107]

uel: 22.2% [51],[32]  
 22.25% [49]  
 22.5% [107]

lel: 1.97% [49],[107]  
 2.0% [51],[32]

Autoign. temp.: 180°C [51],[32],[22],[107]

Flammable liquid. Dangerous fire hazard when exposed to heat or flame. Tends to form explosive peroxides, especially with anhydrides. Emits toxic fumes of CO and CO<sub>2</sub> when heated to decomposition. Flashback along vapor trail can occur. Fight fire with CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [51],[108],[55]

### 318 - 1,4-Dioxane

**Incompatibility:** Oxygen; oxidizing agents; halogens; reducing agents; moisture; heat;  $H_2$  + Raney Ni;  $AgClO_4$ . **WARNING:** anhydrous 1,4-dioxane may form explosive peroxides. Distillation, evaporation, or exposure to light will accelerate peroxide formation [51],[55]

**Handling:** Keep away from heat, sparks, and open flame. **WARNING:** avoid all contact with this substance. Do not breathe vapor or mist (appropriate respirator or wear self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (rubber gloves, laboratory coat, face shield). Use good ventilation (fume hood). Employees should wash promptly when skin is wet or contaminated. Remove clothing immediately if wet or contaminated to prevent fire hazard. Safety shower and eye bath stations should be provided. Keep container tightly closed. Store under nitrogen. Store in a cool, dry, flammable liquid storage area. Store in secure poison area or cabinet. [56],[57],[55]

**Health effects:** 1,4-Dioxane is toxic and a carcinogen. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include liver, kidneys, skin, and eyes. Repeated exposures to low concentrations has resulted in human fatalities, the organs chiefly effected are the liver and kidneys. Acute exposures result in irritation to the eyes and naso-pharynx followed by headache, drowsiness, dizziness, and occasionally nausea and vomiting. Chronic exposures result in loss of appetite, pain and tenderness in the abdomen, malaise, and enlargement of the liver. Further exposure result in suppression of urine, followed by uremia and death. [51]

**Toxicity:** High.

TWA: 25 ppm (90 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: 1 ppm (3.6 mg/m<sup>3</sup>) for 30 min [51]

IDLH: 200 ppm (720 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 2.7-170 ppm (9.7-615 mg/m<sup>3</sup>) [32]

172 ppm (620 mg/m<sup>3</sup>) [107],[104]

Carcinogenicity: animal positive rat and mouse; listed as a carcinogen by the EPA [51],[108],[107],[56],[104]

Mutagenicity: an experimental equivocal tumorigenic agent [51],[55]

**Exposure:**

**External:**

Non-lethal: >200 ppm (720 mg/m<sup>3</sup>) -- noted irritation of eyes [32]

300 ppm (1080 mg/m<sup>3</sup>) for 15 min -- mild irritation of eyes, nose, throat [32]

Lethal: unknown

**Oral:** Unknown

**Inhalation:**

Short-term Inhalation Limits: 100 ppm (360 mg/m<sup>3</sup>) for 60 min [107]

Non-lethal: 470 ppm (1700 mg/m<sup>3</sup>) for 3 days -- toxic effects [51]

5500 ppm (19.8 g/m<sup>3</sup>) for 1 min -- eye effects [51]

Lethal: 208-650 ppm (750-2340 mg/m<sup>3</sup>) for 1 week in unventilated room -- death of an adult human [49]

## Dioxins (TCDD)

 $C_{12}H_4Cl_4O_2$ 

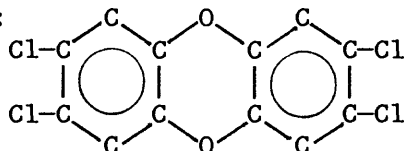
CAS RN: 1746-01-6

Syn: Dioxins (TCDD) \* Dibenzo[b,e][1,4]dioxin, 2,3,7,8-tetrachloro- \*  
 Dioxin \* Dioxin (herbicide contaminant) \* Dioxine\* NCI-C03714 \* TCDBD \*  
 TCDD \* 2,3,7,8-TCDD \* 2,3,7,8-Tetrachloro-dibenzo(b,e)(1,4)dioxan \*  
 2,3,7,8-Tetrachloro-dibenzo-p-doixin \* 2,3,7,8-Tetrachloro-dibenzo-1,4-  
 dioxin \* Tetradioxin \*

Molecular formula:  $Cl_2C_6H_2-O_2-C_6H_2Cl_2$ 

Polychlorinated Polycyclic Hydrocarbon

Structural formula:



Physical properties:

Relative molecular mass:	321.975	
Specific gravity:	unknown	
Boiling point:	500.°C decomposes	[56]
	412.2°C (est)	[41]
Melting point:	305.°C	[51]
	302.°-305°C	[56]
	305.°-306°C	[104]
	295.°C	[59]
Refractive index:	unknown	
Vapor pressure:	3.6x10 <sup>-11</sup> kPa @ 15°C (2.7x10 <sup>-10</sup> mm)	[41]
	8.5x10 <sup>-11</sup> @ 20°C (6.4x10 <sup>-10</sup> mm)	[41]
	1.8x10 <sup>-10</sup> @ 25°C (1.4x10 <sup>-9</sup> mm)	[41]
	2.3x10 <sup>-7</sup> @ 25°C (1.7x10 <sup>-6</sup> mm)	[31]
	4.7x10 <sup>-10</sup> @ 30°C (3.5x10 <sup>-9</sup> mm)	[41]
	2.17x10 <sup>-9</sup> @ 40°C (1.63x10 <sup>-8</sup> mm)	[41]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	

### 320 - Dioxins (TCDD)

Heat of vaporization:	unknown	
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	unknown	
Heat of combustion:	unknown	
Heat of formation:	unknown	
Gibbs (free) energy:	130. kJ/mol (gas) (calc)	[59]

Analytical chemistry: $pP_{oct}$ =	7.02	[59]
	6.83	[31]
	6.64	[27]
	5.38 - 6.64	[41]
	4.37	[12]
$pK_s$ =	NA	
$pK_a$ =	NA	[31]
$pK_{BH}$ =	NA	
Henry's law constant =	$5.47 \times 10^{-21}$ kPa-m <sup>3</sup> /mol (calc)	[41]
	0.000086 dimensionless	[59]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water. Soluble in fats, oils and other nonpolar solvents. [8],[41]

0.2 ppb in water	[41]
0.0193 ppb in water @ 22°C	[41]

Form: White to colorless crystalline solid or needles. [104],[56]

Use: TCDD and other polychlorinated dibenzo-*p*-dioxins are contaminants formed during the production of 2,4,5-TCP, 2,4,5-T (2,4,5-trichlorophenoxyacetic acid) and other chlorophenols. TCDD is formed by the alkaline hydrolysis of 1,2,4,5-tetrachlorobenzene. It has no particular use. It is a contaminant in herbicide formulations. [56]

Fire and explosion hazard: Unknown

Flash point: unknown  
l<sub>el</sub>: unknown  
Autoign. temp.: unknown

Incompatibility: Unknown

Handling: WARNING: avoid all contact. Any possibility of physical contact with this substance should be avoided. Use of gloves, goggles, respirator, full protective clothing, and decontamination after handling is required. Avoid any procedure which will allow TCDD into the environment. Burn contaminated items. Store in a secure poison facility. [56]



**Health effects:** TCDD is the most toxic of the dioxins and one of the most toxic substances known. The toxicity of a dioxin varies with the position and number of chlorines attached to the aromatic rings. Routes of entry are skin absorption, inhalation, ingestion, and eye and skin contact. Points of attack include skin, liver, and central nervous system. Exposure in small doses can cause chloracne, cirrhosis of the liver, personality changes, spontaneous abortion, and birth defects. Also, large doses can cause severe liver damage, coma, and death. Death can follow a lethal dose by weeks. Three ounces could kill the population of New York City. It is a very potent acute and chronic hepatic poison and carcinogen.  
[5],[51],[92]

**Toxicity:** Very High

TWA: no values set [1]

STEL: no values set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: high; a potent carcinogen [51],[56]  
positive in small animals [26]

Mutagenicity: high [104]

**Exposure:** Unknown

## 322 - Endrin

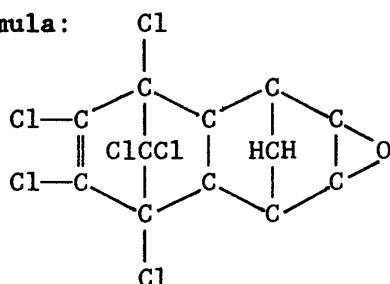
Endrin

 $C_{12}H_8Cl_6O$ 

CAS RN: 72-20-8

Syn: Endrin \* 2,7:3,6-Dimethanonaphth[2,3-b]oxirene, 3,4,5,6,9,9-hexachloro-1a,2,2a,3,6,6a,7,7a-octahydro-(1a $\alpha$ ,2 $\beta$ ,2a $\beta$ ,3 $\alpha$ ,6 $\alpha$ ,6a $\beta$ ,7 $\beta$ ,7a $\alpha$ )- \*  
 Compound 269 \* 1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-,endo,endo- \* EN 57 \* Endrex \* Endricol \*  
 ENT 17251 \* Experimental insecticide 269 \* Hexachloroepoxyoctahydro-endo-endo-dimethanonaphthalene \* 1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-1,4-endo-endo-5,8-dimethanonaphthalene \*  
 Hexadrin \* Isodrin epoxide \* Mendrin \* NA 2761 \* NCI-C00157 \* Nendrin \*  
 Oktanex \* RCRA Waste Number P051 \* SD 3419 \*

Structural formula:



Polychlorinated Cyclic Hydrocarbon

## Physical properties:

Relative molecular mass:	380.913	
Specific gravity:	1.65 @ 25°C	[107]
	1.7	[32]
Boiling point:	decomposes at melting point	
Melting point:	245.°C decomposes	[108]
	226.°-230°C	[56]
	200.°C decomposes	[51], [32], [107], [104]
Refractive index:	NA	
Vapor pressure:	2.66x10 <sup>-8</sup> kPa @ 20°C (2x10 <sup>-7</sup> mm)	[32]
	2.66x10 <sup>-8</sup> @ 25°C (2x10 <sup>-7</sup> mm)	

[104], [108]

Vapor density:	NA
Evaporation rate:	NA
Relative dielectric permittivity:	unknown
Loss tangent:	unknown
Relaxation time:	unknown
Thermal conductivity:	unknown
Electrical resistivity:	unknown
Critical temperature:	unknown
Critical pressure:	unknown
Dynamic viscosity:	NA
Kinematic viscosity:	NA
Surface tension:	NA
Contact angle:	NA
Thermal expansion coefficient:	unknown
Compressibility:	NA
Vapor diffusivity:	unknown
Solution diffusivity:	unknown
Electric dipole moment:	unknown
Ionization potential:	unknown
Magnetic volume susceptibility:	unknown
Speed of sound:	unknown

Heat of melting:	unknown
Heat of vaporization:	unknown
Heat of sublimation:	unknown
Heat capacity @ 25°C:	unknown
Heat of combustion:	unknown
Heat of formation:	unknown
Gibbs (free) energy:	unknown

Analytical chemistry:	pP <sub>oct</sub> =	5.6 (calculated)	[104]
		5.339	[41]
		5.16	[41]
		4.56	[27], [41]
		3.54	[31]
		3.209	[41]
	pK <sub>s</sub> =	NA	
	pK <sub>a</sub> =	NA	
	pK <sub>BH</sub> =	NA	
	Henry's law constant =	0.00005 kPa·m <sup>3</sup> /mol	[41]
	Hydrolysis half-life =	>1.3x10 <sup>8</sup> sec	[8]

**Electrochemical data:** Unknown

Clay-organic interaction data: Fowker et al. (1960)

**Solubility:** Almost insoluble in water and methanol. Moderately soluble in acetone, benzene, carbon tetrachloride, hexone, xylene, other organic common solvents. [22],[108],[41]

0.000026 wt% in water @ 25°C	[41]
200. ppb in water @ 25°C	[41]
17. wt% in acetone @ 25°C	[108]
13.8 wt% in benzene @ 25°C	[108]
3.3 wt% in CCl <sub>4</sub> @ 25°C	[108]
7.1 wt% in hexane @ 25°C	[108]
18.3 wt% in xylene @ 25°C	[108]

**Form:** Colorless to tan, solid or solution. Mild to nonexistent odor. A stereo isomer of Dieldrin, which is the *endo-exo*-isomer. Technical grade is 95-98% pure. Dry formulations may contain up to 75% endrin; liquid formulations up to 25% endrin in flammable xylene. [32],[107],[104]

**Use:** Insecticide: minor constituent in Dieldrin. [108],[104]

**Fire and explosion hazard:** Very low

Flash point: (OC) &gt;26.7°C (in xylene solution) [107]

uel: 7% (in xylene solution) [107]

1el: 1.1% (in xylene solution) [107]

Autoign. temp.: unknown

Nonflammable solid or combustible solution but dangerous. Toxic gases and vapors (such as hydrogen chloride, other volatile chlorinated compounds, and carbon monoxide) may be released when endrin decomposes. Fight fire with dry chemical powder, alcohol or polymer foam, CO<sub>2</sub>. Water may be ineffective. [32],[107]

**Incompatibility:** Strong oxidizers; strong acids, parathion. [51],[32],[56]

## 324 - Endrin

**Handling:** Avoid heat and flame. Prevent any possible inhalation of dust, mists, or fumes (appropriate respirator or self-contained breathing apparatus). Prevent any possible skin and eye contact (rubber gloves; protective shoes and overclothing; splash-proof chemical goggles). Employees should wash immediately when skin is wet or contaminated. Remove nonimpervious clothing immediately if wet or contaminated. Provide emergency showers and eyewash stations. Store in secure poison area or cabinet. [56],[57]

**Health effects:** Endrin is a poison. Routes of entry are inhalation, ingestion, percutaneous absorption, and eye and skin contact. Points of attack include central nervous system, liver, and gastrointestinal system. Overexposure may cause sudden convulsions, headache, abdominal discomfort, vomiting, agitation, dizziness, sleepiness, weakness, and loss of appetite. Death may occur from oral ingestion. [32]

**Toxicity:** High

TWA: 0.006 ppm (0.1 mg/m<sup>3</sup>) (skin) [1]

STEL: no values set [1]

CL: unknown

IDLH: 13 ppm (200 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: unknown

Carcinogenicity: indefinite; suspected human carcinogen [51],[22]

Mutagenicity: experimental teratogen [51]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: 1 mg/kg body wt -- causes symptoms [51]

Lethal: 6.8 g (0.24 ounces) [5]

Inhalation:

Short-term Inhalation Limits: 0.03 ppm (0.5 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: unknown

Lethal: unknown

## Ethanol



CAS RN: 64-17-5

Syn: Ethanol \* Absolute Ethanol \* Alcohol \* Algrain \* Anhydrol \* Anhydrous alcohol \* Denatured alcohol \* Denatured ethanol \* Dehydrated alcohol \* Cologne spirit \* Cologne spirits (alcohol) (DOT) \* Ethanol 200 proof \* Ethanol solution (DOT) \* Ethyl alcohol \* Ethyl alcohol anhydrous \* Ethyl hydrate \* Ethyl hydroxide \* Fermentation alcohol \* Grain alcohol \* Jaysol \* Jaysol S \* Methylcarbinol \* Molasses alcohol \* NCI-C03134 \* Potato alcohol \* SD alcohol 23-hydrogen \* Spirits of wine \* Spirt \* Tecsol \* UN 1170 (DOT) \*

Molecular formula:  $\text{CH}_3\text{-CH}_2\text{OH}$ 

Aliphatic Alcohol

## Physical properties:

Relative molecular mass:	46.06904	
Specific gravity:	0.7893	[105]
	0.7894	[10]
Boiling point:	78.293°C	[49]
	78.3°C	[10]
	78.5°C	[105]
Melting point:	-114.°C	[10]
	-114.49°C	[49]
	-117.3°C	[105]
Refractive index:	1.36143	[49]
	1.3614 @ 20°C	[10]
	1.3611 @ 20°C	[105]
Vapor pressure:	0.133 kPa @ -31°C (1mm)	[105]
	1.333 @ -2.3°C (10mm)	[105]
	5.333 @ 19.0°C (40mm)	[105]
	5.33 @ 19.3°C (40mm)	[51]
	13.332 @ 34.9°C (100mm)	[105]
	53.329 @ 63.5°C (400mm)	[105]
Vapor density:	1.59	[51]
Evaporation rate:	1.60	[49]
Relative dielectric permittivity:	41.8 @ -60°C	[105]
	25.07 @ 20°C	[20]
	24.55 @ 25°C	[10]
	24.30 @ 25°C	[105]
	22.14 @ 40°C	[20]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.179 W/(m-K) @ -20°C	[20]
	0.174 @ 0°C	[20]
	0.1673 @ 20°C	[105]
	0.132 @ 40°C	[20]
	0.156 @ 60°C	[20]
Electrical resistivity:	7.41 MOhm-m @ 25°C	[10]
Critical temperature:	243.1°C	[10]
	243.0°C	[105]
	240.77°C	[49]
Critical pressure:	6.384 MPa	[105]
	6.380	[10]
	6.148	[49]

## 326 - Ethanol

Dynamic viscosity:	1.773 mPa-s @ 0°C	[105]
	1.466 @ 10°C	[105]
	1.200 @ 20°C	[105]
	1.003 @ 30°C	[105]
	0.834 @ 40°C	[105]
	0.702 @ 50°C	[105]
	0.592 @ 60°C	[105]
	0.504 @ 70°C	[105]
Kinematic viscosity:	2.246 $\mu\text{m}^2/\text{s}$ @ 0°C	
	1.857 @ 10°C	
	1.520 @ 20°C	
	1.271 @ 30°C	
	1.057 @ 40°C	
	0.889 @ 50°C	
	0.750 @ 60°C	
	0.639 @ 70°C	
Surface tension:	24.05 mN/m @ 0°C air	[105]
	23.61 @ 10°C vapor	[105]
	22.75 @ 20°C vapor	[105]
	21.89 @ 30°C vapor	[105]
Contact angle: [18]		
	sessile    advancing    receding	
quartz	0            0            0	
calcite	9            13            0	
biotite	0            0            0	
Ca-mont.	swelled    0            swelled	
Thermal expansion coefficient:	0.001096 K <sup>-1</sup>	[49]
Compressibility:	0.963 nPa <sup>-1</sup> @ 0°C	[105]
	1.030 @ 10°C	[105]
	1.098 @ 20°C	[105]
	1.180 @ 30°C	[105]
	1.261 @ 40°C	[105]
	1.360 @ 50°C	[105]
Vapor diffusivity:	10.2 $\mu\text{m}^2/\text{s}$ @ 0°C	[47]
Solution diffusivity:	1.28 nm <sup>2</sup> /s in Water	[47]
Electric dipole moment:	5.64x10 <sup>-30</sup> C-m	[105]
Ionization potential:	10.49 eV (PI)	[105]
Magnetic volume susceptibility:	-7.23x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	1232.1 m/s @ 0°C	[20]
	1196.7 @ 10°C	[20]
	1161.8 @ 20°C	[20]
	1207. @ 25°C	[105]
	1127.6 @ 30°C	[20]
	1094.1 @ 40°C	[20]
	1061.2 @ 50°C	[20]
Heat of melting:	4.187 kJ/mol	[10]
	5.021	[105]
Heat of vaporization:	38.75 kJ/mol	[10]
	40.503	[105]
Heat of sublimation:	42.33 kJ/mol	[10]

Heat capacity @ 25°C:	0.1120 kJ/(mol-K)	(liq)	[10]
	0.1115	(liq)	[105]
	0.0655	(gas)	[10]
	0.0657	(gas)	[105]
Heat of combustion:	-1366.8 kJ/mol @ 25°C	(liq)	[49]
	-1367.7	(liq)	[105]
	-1409.4	(gas)	[49]
Heat of formation:	-277.2 kJ/mol @ 25°C	(liq)	[10]
	-277.87	(liq)	[105]
	-234.6	(gas)	[10]
	-235.26	(gas)	[105]
Gibbs (free) energy:	-174.3 kJ/mol @ 25°C	(liq)	[10]
	-171.7	(liq)	[105]
	-168.0	(gas)	[10]
	-168.7	(gas)	[105]
Analytical chemistry: p <sub>Poct</sub>	0.10		[21]
	-0.15		[21]
	-0.30		[21]
	-0.32		[21]
	-0.31		[24]
	pK <sub>s</sub> = 19.1		[49]
	pK <sub>a</sub> = 15.9 @ 25°C		[10], [49], [24]
	pK <sub>BH</sub> = -1.94 @ 25°C in aqueous H <sub>2</sub> SO <sub>4</sub>		[49]
	Henry's law constant = 0.000637 kPa-m <sup>3</sup> /mol		[24]
	Hydrolysis half-life = unknown		

Electrochemical data: Meites et al. (1983).

Clay-organic interaction data: Ethanol has been reported to both increase and decrease hydraulic conductivity of clay soils (Mesri and Olson, 1971; Griffin et al., 1984). Displacement of water by ethanol in the primary hydration shell around Ca<sup>2+</sup>, Cu<sup>2+</sup> and Al in montmorillonite. Infra-red spectra of Cu-montmorillonite and its complexes with ethanol under various conditions. Basal spacings of montmorillonite samples containing Na<sup>+</sup>, K<sup>+</sup>, Ca<sup>2+</sup> and increasing proportions of Li<sup>+</sup> after heat treatment to 493K for 24 hours and solvation with ethanol (see also [18]). Interlayer complexes of halloysite with ethanol. Complexes formed with rehydrated halloysite obtained by washing the potassium acetate complex with water. Interaction energies for cation-ethanol dipole systems. Butadiene from ethanol caused by organic reaction with clay (Theng, 1974). Also see Barshad, 1952; Bissada, 1967; Brindley et al., 1969; Dandy and Nadiye-Tabbiruk, 1982; Dowdy and Mortland, 1967; Griffin et al., 1984; Mesri and Olson, 1971; Mortland, 1970; Stul, 1985.

Solubility: Soluble in benzene. Miscible with water, ether, acetone, chloroform, and with many organic liquids. [22],[51]

Form: Clear, colorless liquid. Characteristic fragrant odor. Burning taste. Very mobile. Absorbs water rapidly from air. The materials used for denaturing industrial grades contribute substantially to the toxicity and are not taken into account here. [51]

## 328 - Ethanol

**Use:** Most is used in alcoholic beverages in diluted form; solvent in laboratory and industry; manufacture of denatured alcohol, pharmaceuticals (rubbing compounds, lotions, tonics, colognes); in perfumes; in organic synthesis; topical anti-infectants; as an antiseptic; dehydrating agent; octane booster in gasoline. [104],[56]

**Fire and explosion hazard:** High.

Flash point: (CC) 13.11°C [51]

uel: 19.0% @ 60°C [51],[105]

lel: 3.3% @ 60°C [51],[105]

Autoign. temp.: 422.78°C [51]

Highly flammable liquid with low flash point. Dangerous fire hazard when exposed to heat or flame. Moderate explosion hazard when exposed to flame. Fight fire with alcohol or polymer foam, CO<sub>2</sub> or dry chemical. Can use water spray to "knock down" vapor. [51]

**Incompatibility:** Acetyl chloride; (Ag<sub>2</sub>O+NH<sub>4</sub>OH); BrF<sub>5</sub>; Ca(OCl)<sub>2</sub>; ClO<sub>3</sub>; CrO<sub>3</sub>; Cr(OCl)<sub>2</sub>; (cyanuric acid + H<sub>2</sub>O); H<sub>2</sub>O<sub>2</sub>; HNO<sub>3</sub>; (H<sub>2</sub>O<sub>2</sub> + H<sub>2</sub>SO<sub>4</sub>); (I+CH<sub>3</sub>OH + HgO); disulfuryl difluoride; oxidants; platinum; potassium; potassium-tert-butoxide; silver nitrate; silver oxide; [Mn(ClO<sub>4</sub>)<sub>2</sub> + 2;2-dimethoxy propane]; Hg(NO<sub>3</sub>)<sub>2</sub>; HClO<sub>4</sub>; perchlorates; (H<sub>2</sub>S<sub>2</sub>SO<sub>4</sub> + permanganates); HMnO<sub>4</sub>; KO<sub>2</sub>; KOC(CH<sub>3</sub>)<sub>3</sub>; (Ag+HNO<sub>3</sub>); AgNO<sub>3</sub>; AgClO<sub>4</sub>; NaH<sub>3</sub>N<sub>2</sub>; UO<sub>2</sub>(ClO<sub>4</sub>)<sub>2</sub>. [51]

**Handling:** Keep away from heat, sparks and flame. Avoid prolonged inhalation of mist or vapors (appropriate respirator or self-contained breathing apparatus). Avoid eye and skin contact (neoprene, rubber, nitrile, butyl synthetic latex, polyethylene vinyl plastic or PVC coated nylon gloves; lab coat; splash-proof chemical goggles or face shield). Use in well-ventilated area (fume hood). Keep containers tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet. Store in secure poison area. [57]

**Health effects:** Ethanol is toxic. Routes of entry are inhalation of vapor, percutaneous absorption, ingestion, and eye and skin contact. Points of attack include central nervous system, liver, gastrointestinal system, upper respiratory tract, and eyes. It is rapidly oxidized in the body to carbon dioxide and water. Though possessing narcotic properties, sufficient concentrations to produce narcosis are not reached in industry. Large doses can cause alcohol poisoning, and if prolonged over many years cirrhosis of the liver. Repeated ingestions can lead to alcoholism. It is a CNS depressant and causes teratogenic effects, gastrointestinal tract effects, and endocrine glandular effects. It is an equivalent tumorigenic agent. [51],[56]

**Toxicity:** Low.

TWA: 1000 ppm (1900 mg/m<sup>3</sup>) [1]

STEL: no values set [1]

CL: unknown

IDLH unknown

Peak: unknown

Odor threshold: 10-5100 ppm (19-9600 mg/m<sup>3</sup>) [104]

Carcinogenicity: unknown

Mutagenicity: teratogenic effects, equivalent tumorigenic agent [51]



**Exposure:****External:**

Non-lethal: 20 ppm (38 mg/m<sup>3</sup>) in eye -- irritation [51]  
5000-10000 ppm (9400-19,000 mg/m<sup>3</sup>) -- irritation to eyes  
and mucous membranes [51]  
5000-10000 (9400-19,000 mg/m<sup>3</sup>) for 1 hr -- stupor and  
drowsiness [51]

Lethal: unknown

**Oral:**

Non-lethal: 50 mg/kg body wt -- gastrointestinal tract effects in an  
adult male [51]  
1.430 mg/kg body wt -- CNS effects in an adult male [51]  
256 g/kg body wt for 12 wks -- effects on endocrine  
glandular system in an adult female [51]  
5-15 g/kg body wt -- 50% chance of death [107]

Lethal: unknown

**Inhalation:**

Short-term Inhalation Limits: 5000 ppm (9400 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: unknown

Lethal: unknown

## 330 - Ethylbenzene

Ethylbenzene

C<sub>8</sub>H<sub>10</sub>

CAS RN: 100-41-4

Syn: Ethylbenzene \* Benzene, ethyl \* EB \* Ethyl benzene \* Ethylbenzol \*  
 NCI-C56393 \* Phenylethane \* UN 1174 (DOT)

Molecular formula: C<sub>6</sub>H<sub>5</sub>-CH<sub>2</sub>CH<sub>3</sub>

Monocyclic Aromatic Hydrocarbon

## Physical properties:

Relative molecular mass:	106.167	
Specific gravity:	0.8670	[47], [22], [104], [10], [107], [105]
	0.8669	[51]
	0.865	[32]
Boiling point:	136.2°C	[104], [10], [105], [107], [51]
	136.193°C	[49]
	136.187°C	[22]
	136.°C	[32], [56]
Melting point:	-94.4°C	[47]
	-94.9°C	[51]
	-94.97°C	[104], [105]
	-94.975°C	[22], [49]
	-95.°C	[106], [10], [107]
Refractive index:	1.49594	[22]
	1.4959	[106], [10], [105]
	1.49588	[49]
Vapor pressure:	0.1333 kPa @ -9.8°C	(1mm) [105]
	0.666 @ 13.9°C	(5mm) [47], [20]
	0.947 @ 20°C	(7.1mm) [104], [32]
	1.27 @ 25°C	(9.53mm) [23]
	1.333 @ 25.9°C	(10mm) [49], [105], [51]
	1.600 @ 30°C	(12mm) [104]
	5.333 @ 52.8°C	(40mm) [105]
Vapor density:	3.66	[104], [51], [32]
Evaporation rate:	0.89	[49]
	<1.	[32]
Relative dielectric permittivity:	2.412 @ 20°C	[105]
	2.41 @ 20°C	[10]
	2.4042 @ 20°C	[49]
	2.238 @ 25°C	[14]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.132 W/(m-K) @ 20°C	[105]
	0.149 @ 30°C	[47]
	0.142 @ 60°C	[47]
Electrical resistivity:	NA	
Critical temperature:	344.°C	[49]
	343.94°C	[10]
	343.9°C	[105], [107]
Critical pressure:	3.74 MPa	[105]
	3.61	[107]
	3.609	[10]
	3.606	[49]

Dynamic viscosity:	0.691 mPa-s @ 17°C	[105]	
	0.6783 @ 20°C	[49]	
	0.678 @ 20°C	[10]	
	0.6373 @ 25°C	[49]	
	0.64 @ 25°C	[22]	
Kinematic viscosity:	0.797 μm²/s @ 17°C		
	0.7824 @ 20°C		
	0.782 @ 20°C		
	0.7351 @ 25°C		
	0.750 @ 25°C		
Surface tension:	29.20 mN/m @ 20°C vapor	[107], [105]	
	29.05 @ 20°C	[49]	
	28.48 @ 25°C	[49]	
	27.93 @ 30°C	[14]	
	26.79 @ 40°C	[14]	
Contact angle:	[18]		
	sessile	advancing	receding
quartz	12	13	5
calcite	20	18	7
biotite	12	14	5
Ca-mont.	6	swelled	swelled
Thermal expansion coefficient:	unknown		
Compressibility:	0.865 nPa <sup>-1</sup>	[49]	
Vapor diffusivity:	6.58 μm²/s @ 0°C	[47]	
	7.6	[59]	
Solution diffusivity:	0.90 nm²/s	[59]	
Electric dipole moment:	1.968x10 <sup>-30</sup> C-m	[105], [10]	
	1.234x10 <sup>-30</sup> C-m	[49]	
Ionization potential:	8.76 eV (PI)	[105]	
Magnetic volume susceptibility:	-7.968x10 <sup>-6</sup> SI units @20°C	[105]	
Speed of sound:	1351. m/s @ 20°C	[105]	
Heat of melting:	9.190 kJ/mol	[10]	
	9.184	[49]	
Heat of vaporization:	38.943 kJ/mol	[105]	
	35.588	[10]	
	35.57	[107]	
	35.20 @ (bp)	[49]	
	42.25 @ 25°C	[49]	
Heat of sublimation:	42.29 kJ/mol	[10]	
Heat capacity @ 25°C:	0.1863 kJ/(mol-K)	(liq)	[105]
	0.185572	(liq)	[49]
	0.12841	(gas)	[49]
	0.1285	(gas)	[10], [105]
Heat of combustion:	-4567.9 kJ/mol @ 25°C	(liq)	[20]
	-4564.	(liq)	[49]
	-4610.21	(gas)	[22]
	-4568.	@ 20°C (liq)	[105]
Heat of formation:	-12.48 kJ/mol @ 25°C	(liq)	[10]
	-12.456	(liq)	[49]
	-12.35	(liq)	[20]
	29.89	(gas)	[20]
	29.81	(gas)	[10]

### 332 - Ethylbenzene

Gibbs (free) energy: 130.67 kJ/mol @ 25°C (liq) [10]  
80.01 (gas) [10]

Analytical chemistry:  $pP_{oct}$  = 3.34 [31]  
3.15 [104], [8], [21], [59]  
 $pK_s$  = unknown  
 $pK_a$  = 4.35 [105]  
>15. [59]  
 $pK_{BH}$  = unknown  
Henry's law constant = 0.67 kPa-m<sup>3</sup>/mol [41]  
0.6534 [41]  
0.880 @ 25°C [41]  
0.37 dimensionless [59]  
Hydrolysis half-life = NA [8]

Electrochemical data: Neikam et al. (1964), Sasaki et al. (1967), Meites and Zuman (1977), Lund (1983a)

Clay-organic interaction data: Chiou et al. (1983), Rao et al. (1988) [18].

Solubility: Insoluble in NH<sub>3</sub>. Practically insoluble in water. Soluble in ethanol, SO<sub>2</sub>, carbon tetrachloride. Very soluble in ether. Miscible with chloroform, benzene. [51], [32], [10], [47], [104], [49]

0.01 vol% in water @ 15°C [47]  
0.0140 wt% in water @ 15°C [104]  
0.0152 wt% in water @ 20°C [104], [8]  
0.015 wt% in water @ 25°C [10]  
0.0152 wt% in water @ 25°C [49]  
0.0161 wt% in water @ 25°C [23]  
0.0206 wt% in water @ 30°C [104]

Form: Colorless liquid. Pungent, aromatic, gasoline-like odor. [51], [56]

Use: For conversion to styrene monomer; during spray application of vinyl resin surface coating; liberation during manufacture of paints, varnishes, and other surface coatings, during oven baking and drying of surface coatings, during use as an intermediate in dye manufacture, and during production of acetophene by oxidation of ethylbenzene; manufacture and application of rubber adhesives; during electroplating of aluminum on copper or steel; as a heat transfer medium; manufacture of cellulose acetate, styrene, synthetic rubber; present in mixed xylenes; as a dielectric; naphtha constituent; anti-knock agent especially in airplane fuels; 4.6 wt% in gasoline (high octane number). 18th highest volume chemical produced in U.S. (1979). [56], [104]

**Fire and explosion hazard:** High.

Flash point: (CC) 18°C [49]  
 (CC) 15°C [32],[51],[107],[22]  
 (OC) 26.7°C [107]

uel: 6.8% [51]  
 6.7% [32],[107]

lel: 1.2% [51]  
 1.0% [32],[107]

Autoign. temp.: 460°C [107]  
 432°C [51],[32],[22]

Highly flammable liquid. Dangerous. Keep away from heat and open flame. Flash back along vapor trail can occur. Can react vigorously with oxidizing materials. Fire emits toxic gases and vapors, such as CO and CO<sub>2</sub>. Fight fire with alcohol or polymer foam (most effective), CO<sub>2</sub>, dry chemical powder. Can use water spray to "knock down" vapor. [51],[55]

**Incompatibility:** Strong oxidizing materials. [51],[56]

**Handling:** Keep away from heat, sparks, and open flame. Avoid breathing vapor or mist (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, on clothing (chemical resistant gloves and over clothing [butyl synthetic latex, polyethylene and polyurethane coated nylon are best but still provide only marginal protection], goggles or face shield). Use in well-ventilated area (fume hood). Safety shower and eye bath stations should be available. Keep container tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet. [57],[107],[32],[55]

**Health effects:** Ethylbenzene is an irritant. Routes of entry are inhalation, ingestion, and eye and skin contact. Points of attack include eyes, upper respiratory tract, skin, and central nervous system. Both liquid and vapor are irritating to eyes, skin, mucous membranes, and upper respiratory tract. Erythema and inflammation of the skin may result from contact of the skin with the liquid. Exposure to the vapor causes lachrymation and irritation of the nose and throat, dizziness, and a sense of constriction of the chest. The irritation is sufficient to cause workers to leave an atmosphere containing 0.5% of the vapor. Narcotic in high concentrations. Liver, kidney and pancreatic damage are also possible. [51],[56],[55],[74]

**Toxicity:** Moderate.

TWA: 100 ppm (435 mg/m<sup>3</sup>) (skin) [1]  
 STEL: 125 ppm (545 mg/m<sup>3</sup>) [1]  
 IDLH: 2000 ppm (8700 mg/m<sup>3</sup>) [107],[56]  
 Odor threshold: 0.25-200 ppm (1-870 mg/m<sup>3</sup>) [104]  
 0.46-0.6 ppm (2-2.6 mg/m<sup>3</sup>) [104]  
 140 ppm (608 mg/m<sup>3</sup>) [107],[32]

**Carcinogenicity:** unknown

**Mutagenicity:** experimental teratogen [51]

### 334 - Ethylbenzene

#### Exposure:

##### External:

Non-lethal: 200 ppm (870 mg/m<sup>3</sup>) -- eye irritation [32]  
1000 ppm (4350 mg/m<sup>3</sup>) -- irritant to the eyes [51]  
2000 ppm (8700 mg/m<sup>3</sup>) -- extreme irritation, dizziness,  
irritation of the nose and throat, sense of constriction  
in the chest [51]

Lethal: unknown

Oral: unknown

##### Inhalation:

Short-term Inhalation Limits: 200 ppm (870 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: unknown

Lethal: unknown

Ethylene glycol

 $C_2H_6O_2$ 

CAS RN: 107-21-1

Syn: Ethylene glycol \* 1,2 Ethanediol \* 1,2 Dihydroxyethane \* Ethylene alcohol \* Ethylene dihydrate \* Fridex \* Glycol \* Glycol alcohol \* 2-Hydroxyethanol \* Macrogol 400 BPC \* Monoethylene glycol \* NCI-C00920 \* Ramp \* Tescol \* Ucar 17 \*

Molecular formula:  $HOCH_2CH_2OH$ 

Polyhydric alcohol

**Physical properties:**

Relative molecular mass:	62.07	
Specific gravity:	1.1135	[10],[49],[104],[108]
	1.1088	[106],[105]
	1.1155	[22],[107]
Boiling point:	197.2°C	[20][22]
	197.4°C	[47]
	197.5°C	[49],[51]
	197.6°C	[10],[107],[108]
	198.°C	[104],[105]
	198.93°C	[106]
Melting point:	-11.5°C	[106],[105]
	-12.6°C	[49]
	-13.°C	[10],[51],[107],[108]
	-15.6°C	[47],[22]
	-17.4°C	[20]
Refractive index:	1.4318 @ 20°C	[49],[106],[105]
	1.4319 @ 20°C	[10]
Vapor pressure:	0.0067 kPa @ 20°C	(0.05mm) [51],[104]
	0.0117 @ 25°C	(0.088mm) [49]
	0.1333 @ 53°C	(1mm) [105],[47]
	0.667 @ 79.7°C	(5mm) [47]
	1.333 @ 92.1°C	(10mm) [105]
Vapor density:	2.14	[51],[104]
Evaporation rate:	unknown	
Relative dielectric permittivity:	37.7 @ 25°C	[10],[11],[49],[105]
	38.7 @ 20°C	[20],[108]
	39.4 @ 30°C	[49]
	34.9 @ 40°C	[20]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.2611 W/(m-K) @ 20°C	[105]
	0.2660 @ 0°C	[10]
	0.2648 @ 0°C	[47]
Electrical resistivity:	0.033 MOhm-m @ 25°C	[10],[11]
	0.00862 @ 25°C	[49]
Critical temperature:	NA	[107]
Critical pressure:	NA	[107]

### 336 - Ethylene glycol

Dynamic viscosity:	26.09 mPa-s @ 15°C	[10], [49], [108]	
	19.9 @ 20°C	[105]	
	21. @ 20°C	[108]	
	17.3 @ 25°C	[108]	
	13.76 @ 30°C	[49]	
	9.13 @ 40°C	[105]	
	4.95 @ 60°C	[105]	
	3.02 @ 80°C	[105]	
	1.99 @ 100°C	[105]	
Kinematic viscosity:	23.43 μm²/s @ 15°C		
	17.87 @ 20°C		
	18.86 @ 20°C		
	15.54 @ 25°C		
	12.36 @ 30°C		
	8.20 @ 40°C		
	4.45 @ 60°C		
	2.71 @ 80°C		
	1.79 @ 100°C		
Surface tension:	50.21 mN/m @ 15°C	[10]	
	48.4 @ 20°C	[49], [108]	
	47.7 @ 20°C	[105]	
	46.24 @ 30°C	[49]	
Contact angle: [18]			
	sessile	advancing	receding
quartz	35	31	4
calcite	72	66	36
biotite	19	24	4
Ca-mont.	13	14	0
Thermal expansion coefficient:	6.26x10 <sup>-4</sup> K <sup>-1</sup> @ 20°C	[49]	
Compressibility:	0.372 nPa <sup>-1</sup> @ 25°C	[105]	
	0.400 @ 45°C	[105]	
	0.432 @ 65°C	[105]	
	0.470 @ 85°C	[105]	
	0.514 @ 105°C	[105]	
Vapor diffusivity:	unknown		
Solution diffusivity:	unknown		
Electric dipole moment:	7.605x10 <sup>-30</sup> C-m	[10], [105]	
	7.705x10 <sup>-30</sup>	[49]	
	7.338x10 <sup>-30</sup>	[108]	
Ionization potential:	unknown		
Magnetic volume susceptibility:	-8.77x10 <sup>-6</sup> SI units @ 20°C	[105]	
Speed of sound:	1658. m/s @ 25°C	[105]	
Heat of melting:	11.64 kJ/mol	[10]	
	11.62	[108]	
	11.24	[47], [105]	
	9.958	[49]	
Heat of vaporization:	67.8 kJ/mol @ 25°C	[49]	
	58.751	[105]	
	50.46 (bp)	[49]	
	49.66	[10], [47]	
	49.636	[108]	
Heat of sublimation:	65.65 kJ/mol	[10]	



Heat capacity @ 19.8°C:	0.1494 kJ/(mol-K)	(liq)	[49]
@ 25°C:	0.1499	(liq)	[10], [105]
	0.0971	(gas)	[10]
@ 27°C:	0.1510	(liq)	[49]
Heat of combustion:	-1190.43 kJ/mol @ 25°C	(liq)	[20]
	-1189.72	(liq)	[49]
	-1180.26 @ 20°C	(liq)	[105]
Heat of formation:	-454.60 kJ/mol @ 25°C	(liq)	[105]
	-454.80	(liq)	[49]
	-455.11	(liq)	[10], [20], [105]
	-389.58	(gas)	[10]
	-451.80	(gas)	[47]
	-387.9	(gas)	[49]
Gibbs (free) energy:	-322.89 kJ/mol @ 25°C	(liq)	[105]
	-323.43	(liq)	[10], [105]
	-304.67	(gas)	[10]
	-320.04	(gas)	[47]
Analytical chemistry: $pP_{oct}$ =	-1.93		[104], [21]
	-1.36		[24]
$pK_s$ =	15.84		[49]
$pK_a$ =	14.22		[10], [105]
	14.24		[49]
$pK_{BH}$ =	unknown		
Henry's law constant =	0.000006 kPa-m <sup>3</sup> /mol		[24]
Hydrolysis half-life =	unknown		

**Electrochemical data:** Meites and Zuman (1977)

**Clay-organic interaction data:** Ethylene glycol is reported to both increase and decrease the hydraulic conductivity of clay-soils (Anderson and Brown, 1981; Anderson and Jones, 1983; Dowdy and Mortland, 1968; Greenland, 1972; Griffin et al., 1984; Lord et al., 1983; Mortland, 1970; Parfitt and Greenland, 1970; Schramm et al., 1986). Ethylene glycol intercalates clay minerals causing some clays to expand, enhancing the identification of clay mineralogy and determining the surface area of the clay. As a result ethylene-glycol-clay interactions are one of the most heavily studied of clay-organic reactions (Brindley, 1966; Theng, 1974; Hoffman and Brindley, 1961; Reynolds, 1965; Walker, 1958).

**Solubility:** Soluble in ether and chloroform. Slightly soluble in benzene. Very soluble in ethanol, acetone, glycerol, acetic acid. Miscible with water. [105], [10], [47], [24]

1.0 wt% in ether [10], [47]

**Form:** Colorless, slightly viscous, bittersweet tasting liquid. Hygroscopic, absorbing twice its weight of water at 100% relative humidity. Has a tendency to supercool. [51], [108]

### 338 - Ethylene glycol

**Use:** As antifreeze in cooling and heating systems and in deicing fluids for airport runways; in hydraulic brake fluids; as an industrial humectant; an ingredient in electrolytic condensers; solvent in the paint and plastics industries; used in the formulation of printers' inks; a softening agent for cellophane and a stabilizer for soybean foam used to extinguish oil and gasoline fires; in synthesis of safety explosives, glyoxal, alkaloid resins, plasticizers, elastomers, synthetic fibers, synthetic waxes, and pharmaceuticals. [108],[22],[56]

**Fire and explosion hazard:** Low

Flash point: (CC) 111.2°C [51],[107]  
(OC) 116.°C [49],[22],[107]  
(OC) 115.°C [108]

uel: NA [107]

lcl: 3.2% [51],[107]

Autoign. temp.: 400°C [51]  
412.8°C [107]  
413°C [49],[22]

Slightly flammable liquid. Can be explosive when exposed to flame. Extinguish fire with water fog, alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder. Water or foam may cause frothing. [107]

**Incompatibility:** Chlorosulfonic acid; oleum; H<sub>2</sub>SO<sub>4</sub>; HClO<sub>4</sub>; P<sub>2</sub>S<sub>5</sub>. [51]

**Handling:** Avoid heat and flame. Avoid prolonged inhalation (appropriate respirator or self-contained breathing apparatus). Avoid skin and eye contact (protective overclothing and gloves; splash-proof safety goggles). Wash skin if contaminated. Store in cool, dry, well-ventilated, secure poison area or cabinet. [107],[56],[53]

**Health effects:** Ethylene glycol is poisonous. Routes of entry are inhalation of particulate or vapor, ingestion, and percutaneous absorption. Points of attack include the central nervous system. When ingested it has a narcotic effect by first stimulating the central nervous system followed by depression, vomiting, drowsiness, coma, respiratory failure, convulsions, renal damage, and death. Poisoning resulting from vapor usually occurs only if the liquid is heated or is in particulate form. [56],[108],[49],[51]

**Toxicity:** Moderate

TWA: no value set [1]

STEL: no value set [1]

CL: 50 ppm (125 mg/m<sup>3</sup>) [1]

IDLH: unknown

Peak: unknown

Odor threshold: NA [107]

Carcinogenicity: none [104]

Mutagenicity: none [104]

**Exposure:**

External:

Non-lethal: nearly harmless to skin [107]

Lethal: NA [107]

Oral:

Non-lethal: 7400 mg/kg body wt -- systemic damage in a child [51]

Lethal: 1.4 ml/kg body wt -- death of an adult male [104],[108]

710 mg/kg body wt -- death of an adult human [51]

1637 mg/kg body wt -- death of an adult male [51]

Inhalation:

Short-term Inhalation Limit: NA [107]

Non-lethal: 3940 ppm -- irritation to respiratory system [51]

Lethal: unknown

## 340 - Ethylene oxide

Ethylene oxide

C<sub>2</sub>H<sub>4</sub>O

CAS RN: 75-21-8

Syn: Ethylene oxide \* Oxirane \* Anprolene \* Dihydrooxirene \* Dimethylene oxide \* EO \* Epoxyethane \* 1,2-Epoxyethane \* Ethene oxide \* ETO \* NCI-C50088 \* Oxacyclopropane \* Oxane \* Oxidoethane \*  $\alpha,\beta$ -Oxidoethane \* Oxyfume \* Oxyfume 12 \* T-gas \*

Molecular formula: H<sub>2</sub>C-O-CH<sub>2</sub> or CH<sub>2</sub>-CH<sub>2</sub>  
 $\begin{array}{c} \text{---} \end{array}$   $\begin{array}{c} \text{---} \end{array}$   
 $\begin{array}{c} \text{---} \end{array}$   $\begin{array}{c} \text{---} \end{array}$

Aliphatic Cyclic Ether

## Physical properties:

Relative molecular mass:	44.0532	
Specific gravity:	0.869	[107]
	0.8694	[108]
	0.8711 (20/20)	[51], [22]
	0.8824 (10/10)	[105], [106]
Boiling point:	11.°C	[104]
	10.6°C	[10], [107]
	10.7°C	[105], [51], [108]
	10.73°C	[22], [7]
Melting point:	-111.°C	[105], [104], [106], [108]
	-111.3°C	[105], [51], [47], [22]
	-112.5°C	[7]
	-112.6°C	[107]
	-122.44°C	[10]
Refractive index:	1.3597 @ 7°C	[10], [105], [108], [7]
Vapor pressure:	13.32 kPa @ -32.1°C (100mm)	[105], [47]
	26.67 @ -19.5°C (200mm)	[47]
	53.33 @ -4.9°C (400mm)	[105], [47]
	101.3 @ 10.7°C (760mm)	[105], [47]
	146.0 @ 20°C (1095mm)	[51], [104]
	212.8 @ 30°C (1596mm)	[104]
Vapor density:	1.52	[51], [104]
	1.5	[107]
	1.49	[7]
Evaporation rate:	unknown	
Relative dielectric permittivity:	13.9 @ -1°C	[105]
	14. @ -1°C	[11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	196.°C	[107], [10]
	195.8°C	[105], [20], [7]
	192.°C	[47]
Critical pressure:	7.2 MPa	[107], [20], [10]
	7.194	[7]
	7.1	[105]
Dynamic viscosity:	0.577 mPa-s @ -49.8°C	[105]
	0.488 @ -38.2°C	[105]
	0.394 @ -21.0°C	[105]
	0.320 @ 0.0°C	[105], [22]
	0.31 @ 0°C	[7]

Kinematic viscosity:	0.664 $\mu\text{m}^2/\text{s}$ @ -49.8°C	
	0.562 @ -38.2°C	
	0.453 @ -21.0°C	
	0.368 @ 0.0°C	
	0.365 @ 0°C	
Surface tension:	30.8 mN/m @ -20°C	[105]
	27.6 @ 0°C	[105]
	24.3 @ 20°C	[105], [107], [7]
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	6.304x10 <sup>-30</sup> C-m	[105]
Ionization potential:	10.6 eV (PI,S)	[105]
Magnetic volume susceptibility:	-7.77x10 <sup>-6</sup> SI units @ 7°C	[105]
Speed of sound:	unknown	
Heat of melting:	5.177 kJ/mol	[105], [107]
	5.1765	[7]
	5.175	[10]
Heat of vaporization:	25.545 kJ/mol	[107], [7]
	25.544	[10]
	28.5678	[105]
Heat of sublimation:	24.953 kJ/mol	[10]
Heat capacity @ 25°C:	0.0880 kJ/(mol-K) (liq)	[105]
	0.0479 (gas)	[105]
	0.048316 (gas)	[10]
	0.0494 (gas)	[7]
Heat of combustion:	-1264.83 kJ/mol @ 20°C (liq)	[105]
Heat of formation:	-77.87 kJ/mol @ 25°C (liq)	[105]
	-52.670 (gas)	[10], [105]
Gibbs (free) energy:	-11.85 kJ/mol @ 25°C (liq)	[105]
	-13.06 (gas)	[105]
	-13.105 (gas)	[10]
Analytical chemistry:	pP <sub>oct</sub> = -0.30	[23], [21]
	pK <sub>s</sub> = unknown	
	pK <sub>a</sub> = unknown	
	pK <sub>BH</sub> = unknown	
	Henry's law constant = unknown	
	Hydrolysis half-life = 1x10 <sup>6</sup> sec	[13]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Soluble in acetone, benzene. Very soluble in ether. Miscible with water, ethanol. [51], [105], [47], [10]

Form: Colorless liquid (or gas at room temperature). Sweet, olefinic odor. Shipped as liquified gas. Commercial grades must be 100% pure and contain no acetylene. [51], [22], [108]

### 342 - Ethylene oxide

**Use:** Intermediate in organic synthesis for ethylene glycol, polyglycols, glycol ethers, esters, ethanolamines, acrylonitrile, plastics, and surface-active agents; fumigant for foodstuffs and textiles; agricultural fungicide; sterilization for surgical instruments; rocket propellant. [56],[108],[22]

**Fire and explosion hazard:** High

Flash point: (OC) <17.8°C [22],[107]

(OC) -20°C [51]

(OC) -28.9°C [7]

uel: 100% [107],[51],[22],[7],[6]

lel: 3% [107],[51],[22],[7],[6]

Autoign. temp.: 428.9°C [107],[51],[22]

Extremely flammable liquid or gas. Very dangerous fire hazard when exposed to heat or flame. Severe explosion hazard when exposed to flame.

Flashback along vapor trail may occur. May polymerize violently if contaminated with alkaline or acidic materials and metal oxides or chlorides. Fight fire by stopping flow of gas. Use water, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [51],[107]

**Incompatibility:** Strong acids; alkalis; oxidizers; catalytic anhydrous iron chlorides; aluminum chlorides; tin chlorides; iron oxides; aluminum; alcohols; air; m-nitroaniline; ammonia; trimethyl amine; copper; magnesium perchlorate; mercaptans; potassium; alkane thiols; bromoethane. [56],[51]

**Handling:** Keep away from heat, flame, sparks, or other sources of ignition. Avoid inhalation if mist or vapor (appropriate respirator or self-contained breathing apparatus). Avoid any possible eye or skin contact (rubber gloves; laboratory coat; splash-proof goggles or face shield). Wash immediately when skin is wet or contaminated. Remove clothing immediately if wet or contaminated to avoid flammability hazard. Provide emergency shower and eyewash stations. Keep container tightly closed, out of sun, and away from heat. Store in cool, dry, well-ventilated, flammable liquid storage area or cabinet. Cylinder temperature should not exceed 52°C (125°F). [56],[57]

**Health effects:** Ethylene oxide is an irritant. Routes of entry are inhalation of gas, ingestion, and eye and skin contact. Points of attack include eyes, blood, respiratory system, liver, central nervous system, kidneys, and lungs. It is an irritant to the skin, eyes, mucous membranes, and respiratory tract. Skin irritation may lead to severe a dermatitis with blisters, blebs, and burns. Large amounts evaporating from the skin may cause frostbite. Breathing high concentrations can cause nausea, vomiting, irritation to the nose, and unconsciousness. Pulmonary edema may occur. [51],[108],[56]

**Toxicity: High**TWA: 1 ppm (2 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: 75 ppm (135 mg/m<sup>3</sup>) for 15 min [56]IDLH: 800 ppm (1440 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 0.8-500 ppm (1.5-900 mg/m<sup>3</sup>) [104]50 ppm (90 mg/m<sup>3</sup>) [107]

Carcinogenicity: suspected human carcinogen [1],[56]

Mutagenicity: experimental neoplastic effects, teratogen, mutagen [51]

**Exposure:**

## External:

Non-lethal: unknown

Lethal: unknown

## Oral:

Non-lethal: unknown

Lethal: unknown

## Inhalation:

Short-term Inhalation Limits: 200 ppm (360 mg/m<sup>3</sup>) for 30 min [107]Non-lethal: 5-10 ppm (9-18 mg/m<sup>3</sup>) for 10 yrs -- no effects [104]>10 ppm (18 mg/m<sup>3</sup>) -- unsatisfactory conditions [104]100 ppm (180 mg/m<sup>3</sup>) -- symptoms of illness [104]250 ppm (450 mg/m<sup>3</sup>) -- severe toxic effects may occur [104]500 ppm (900 mg/m<sup>3</sup>) for 2 min -- toxic concentration in an adult female [51]12500 ppm (22,500 mg/m<sup>3</sup>) for 10 sec -- irritation [51]

Lethal: unknown

## 344 - Fluoranthene

Fluoranthene

C<sub>16</sub>H<sub>10</sub>

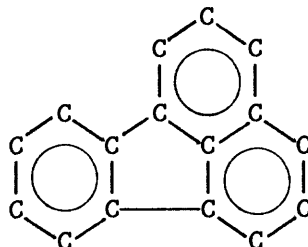
CAS RN: 206-44-0

Syn: Fluoranthene \* 1,2-Benzacenaphthene \* Benzo(*jk*)fluorene \* Idryl \*  
 1,2-(1,8-Naphthylene)benzene \* 1,2-(1,8-Naphthalenediyl)benzene \* RCRA  
 Waste Number U120 \*

Molecular formula: C<sub>16</sub>H<sub>10</sub>

Polynuclear Aromatic Hydrocarbon

Structural formula:



## Physical properties:

Relative molecular mass:	202.255	
Specific gravity:	1.252 @ 0/4	[105], [106], [10]
Boiling point:	367.°C	[51]
	375.°C	[105], [106]
	384.°C	[10]
Melting point:	107.°C	[22], [104]
	107.°-110°C	[10]
	107.8°C	[105]
	111.°C	[56]
	120.°C	[51]
Refractive index:	unknown	
Vapor pressure:	0.0013 kPa @ 20°C (0.01mm)	[51]
	6.7x10 <sup>-7</sup> @ 25°C (5.0x10 <sup>-6</sup> mm)	[31]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	8.54 eV	[41]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	18.871 kJ/mol	[105]
Heat of vaporization:	unknown	
Heat of sublimation:	103.2 kJ/mol	[10]



Heat capacity @ 25°C:	unknown	
Heat of combustion:	unknown	
Heat of formation:	191.5 kJ/mol @ 25°C (sol)	[10]
Gibbs (free) energy:	345.8 kJ/mol @ 25°C (sol)	[10]

Analytical chemistry: $p_{\text{Oct}}$ =	5.33	[8]
	5.22	[41]
	4.90	[31],[59]
$pK_s$ =	NA	
$pK_a$ =	>15.	[59]
	NA	[31]
$pK_{BH}$ =	NA	
Henry's law constant =	1.71 kPa-m <sup>3</sup> /mol @ 25°C	[41]
	0.00026 dimensionless (calc)	[59]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water. Soluble in ethanol, ether, benzene, chloroform, carbon disulfide, glacial acetic acid.  
[105],[106],[10]

0.265 ppm in water @ 25°C	[104]
0.1 ± 0.06 ppm in seawater @ 25°C	[104]

Form: Colorless solid, colored needles, or yellow crystals. [51],[22],[56],[55]

Use: Produced from the pyrolytic processing of organic raw materials such as coal and petroleum at high temperatures. Occurs naturally as a product of plant biosynthesis. It is also contained in cigarette smoke. See [104] for more complete listings of concentrations in gasoline, cigarettes, coal tar pitch, etc. [56],[104]

Fire and explosion hazard: Low.

Flash point: unknown

uel: unknown

lel: unknown

Autoign. temp.: unknown

Slightly flammable solid. Slight fire hazard when exposed to heat or flame. When heated to decomposition it emits acrid smoke and fumes, including CO and CO<sub>2</sub>. Fight fire with water spray, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [51],[55]

Incompatibility: Strong oxidizing agents. [55]

Handling: Do not breathe dust or fumes (appropriate respirator or self-contained breathing apparatus required). Do not get in eyes, on skin, or on clothing (polyvinyl alcohol and viton gloves and suits; safety goggles, other protective clothing). Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [53],[55]

### 346 - Fluoranthene

**Health effects:** Fluoranthene is an irritant and potent cocarcinogen. Routes of entry are ingestion, inhalation, skin absorption, and eye and skin contact. Exposure may cause irritation. Laboratory experiments have shown mutagenic effects. The chemical, physical, and toxicological properties have not been thoroughly investigated. [55],[89]

**Toxicity:** Moderate.

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: does not exhibit properties of a primary carcinogen, but  
it is a potent cocarcinogen [56]

animal no evidence (IARC cancer review) [55]

Mutagenicity: experimental equivocal tumorigenic effects [51]

equivocal tumorigenic agent by RTECS criteria [55]

**Exposure:** Unknown

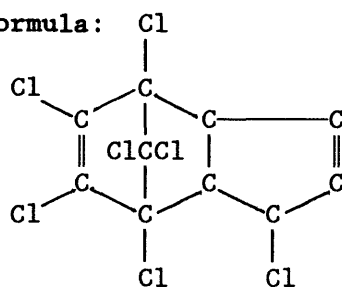
Heptachlor

 $C_{10}H_5Cl_7$ 

CAS RN: 76-44-8

Syn: Heptachlor \* 4,7-Methano-1H-indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro- \* Aahepta \* Agroceres \* Basaklor\* 3-Chlorochlordene \* Drinox H-34 \* E 3314 \* ENT 15152 \* GPKh \* H34 \* Hepta \* Heptachlorane \* 3,4,5,6,7,8,8-Heptachlorodicyclopentadiene \* 3,4,5,6,7,8,8a-Heptachlorodicyclopentadiene \* 1,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-endo-methanoindene \* 1,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindane \* 1,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindene \* Heptachlorodicyclopentadiene \* Heptagran \* Heptagranox \* Heptamak \* Heptamul \* Heptasol \* Heptox \* 4,7-Methanoindene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro- \* NA 2761 \* NCI-C00180 \* RCRA Waste Number P059\* Rhodiachlor \* Soleptax \* Velsicol 104 \* Velsicol heptachlor \*

Structural formula:



Polychlorinated Hydrocarbon

**Physical properties:**

Relative molecular mass:	373.321	
Specific gravity:	1.57-1.59	[105], [104], [22]
	1.57	[106]
	1.66	[107], [105]
	1.65	[32]
Boiling point:	decomposes	[107]
Melting point:	95.°-96°C	[105], [56], [104], [22], [108]
	96.°C	[51]
	46.°-74°C	[107], [32]
Refractive index:	unknown	
Vapor pressure:	$4 \times 10^{-5}$ kPa @ 25°C ( $3 \times 10^{-4}$ mm)	[104], [108]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	unknown	

### 348 - Heptachlor

Ionization potential: unknown  
Magnetic volume susceptibility: unknown  
Speed of sound: unknown  
Heat of melting: unknown  
Heat of vaporization: unknown  
Heat of sublimation: unknown  
Heat capacity @ 25°C: unknown  
Heat of combustion: unknown  
Heat of formation: unknown  
Gibbs (free) energy: unknown

Analytical chemistry:  $pP_{oct}$  = 5.44 [27], [41]  
4.41 [31]  
4.40 [41]  
 $pK_s$  = NA  
 $pK_a$  = NA  
 $pK_{BH}$  = NA  
Henry's law constant = unknown  
Hydrolysis half-life =  $8.6 \times 10^4$  to  $2.6 \times 10^5$  sec [8]

Electrochemical data: Unknown

Clay-organic interaction data: Huang and Liao (1970), Malina et al. (1956)

Solubility: Nearly insoluble in water. Soluble in ethanol, ether, benzene, xylene, organic solvents, acetone, carbon tetrachloride, kerosene, cyclohexanone. [51], [22], [41]

100. ppb @ 15°C [41]  
180. ppb @ 25°C [8], [41]  
315. ppb @ 35°C [41]  
490. ppb @ 45°C [41]

Form: White to light tan, waxy solid crystals. Camphor-like odor.  
Commercial technical grades contains about 72% heptachlor and 28% related compounds. [107], [56], [104]

Use: Insecticide for termite control. [56], [41]

Fire and explosion hazard: Very low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable solid. Dangerous because irritating and toxic hydrogen chloride fumes may form in fire. [51], [107]

Incompatibility: Melted heptachlor with iron or rust. [32], [108], [56]

Handling: Avoid heat and flame. Prevent inhalation of dust, mist, or vapor (appropriate respirator or self contained breathing apparatus). Prevent any possibility of eye or skin contact (protective overclothing; splash-proof chemical goggles; rubber gloves). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [107]

**Health effects:** Heptachlor is highly toxic. Routes of entry are inhalation, skin absorption, ingestion, and eye and skin contact. Points of attack include central nervous system, gastrointestinal tract, liver, skin, and eyes. Inhalation of dust causes irritability, tremors, and collapse. Ingestion causes nausea, vomiting, diarrhea, and irritation of the gastrointestinal tract. Contact with dust causes irritation of eyes and moderate irritation of the skin. Liver damage may develop. Overexposure may stimulate the central nervous system, followed by paralysis and depression. [108],[107],[22]

**Toxicity:** High.

TWA: 0.03 ppm (0.5 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 6.55 ppm (100 mg/m<sup>3</sup>) [56],[107]

Peak: unknown

Odor threshold: 0.02 mg/kg -- detection [104]

0.02 ppm (0.3 mg/m<sup>3</sup>) [107]

Carcinogenicity: positive mouse, negative rat [51]

causes human leukemia and blood dyscrasias [17]

Mutagenicity: positive [37]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: 0.13 ppm (2 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: unknown

Lethal: unknown

## 350 - Hexachlorobenzene

Hexachlorobenzene

 $C_6Cl_6$ 

CAS RN: 118-74-1

Syn: Hexachlorobenzene \* Benzene, hexachloro- \* Amatin \* Anticarie \* Bunt-cure \* Bunt-no-more \* Co-op hexa \* Granox NM \* HCB \* Hexa C.B. \*  
 Hexachlorbenzene \* Julin's carbon chloride \* No Bunt \* No Bunt 40 \* No Bunt 80 \* No Bunt liquid \* Pentachlorophenyl chloride \* Perchlorobenzene \*  
 Phenyl perchloryl \* Sanocide \* Smut-go \* RCRA Waste Number U127 \* Sanocid \* Snieciotox \* UN 2729 (DOT) \*

Molecular formula:  $C_6Cl_6$ 

Polychlorinated Aromatic Halide

## Physical properties:

Relative molecular mass:	284.784	
Specific gravity:	2.044 @ 23°C	[10], [104], [51], [108]
	1.5691 @ 23.6°C	[105]
Boiling point:	323.°-326°C	[10], [51], [56], [108]
	322.°-326°C	[104]
	322.°C sublimes	[105]
Melting point:	231.°C	[10], [51], [56], [108]
	227.°C	[104]
	229.°C	[104]
	230.°C	[105]
Refractive index:	unknown	
Vapor pressure:	1.452x10 <sup>-6</sup> kPa @ 23°C (1.089x10 <sup>-5</sup> mm)	[104]
	1.452x10 <sup>-6</sup> @ 20°C (1.089x10 <sup>-5</sup> mm)	[8]
	0.133 @ 114°C (1mm)	[51], [105]
Vapor density:	9.8	[51]
	9.84	[104]
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	-1.059x10 <sup>-6</sup> SI units @ 24°C	[105]
Speed of sound:	unknown	
Heat of melting	25.54 kJ/mol	[10]
	23.853	[105]
Heat of vaporization:	63.636 kJ/mol	[105]
Heat of sublimation:	97.13 kJ/mol	[10]
Heat capacity @ 25°C:	0.2014 kJ/(mol-K) (sol)	[10]
	0.1733 (gas)	[10]

Heat of combustion:	-2131.0 kJ/mol @ 20°C (sol)	[105]
Heat of formation:	-131.05 kJ/mol @ 25°C (sol)	[10]
	-33.91 (gas)	[10]
Gibbs (free) energy:	1.05 kJ/mol @ 25°C (sol)	[10]
	44.21 (gas)	[10]
Analytical chemistry: $pP_{oct}$ =	6.41	[31]
	6.18	[8]
	5.66	[27]
	5.47	[12]
	5.31	[23]
	4.13	[21]
	5.0 - 6.18	[41]
$pK_s$ =	NA	
$pK_a$ =	NA	[31]
$pK_{BH}$ =	NA	
Henry's law constant =	0.17 kPa-m <sup>3</sup> /mol	[41]
	0.13 @ 23°C	[41]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: None (Dragun and Helling, 1985)

Solubility: Almost insoluble in water. Soluble in benzene, chloroform, hot ether. Very soluble in hot ethanol. [22],[108],[104]

0.0004-0.0006 wt% in water [104],[8]

0.011 wt% (99% pure) in water @ 24°C

[104]

Form: A white crystalline monoclinic solid. [104],[51],[56],[108]

Use: HCB is manufactured and formulated for application to seed wheat to prevent bunt; most of the HCB in the environment comes from agricultural processes. HCB is used as a starting material for the production of pentachlorophenol which is marketed as a wood preservative; one of the main substances in the tarry residue which results from the production of chlorinated hydrocarbons; a by-product in the production of chlorine gas by the electrolysis of sodium chloride using a mercury electrode; fungicide; in organic synthesis; manufacturing of ordnance and pyrotechnics, sodium chlorate, aluminium, vinyl chloride, graphite electrode, synthetic rubber. [56],[108]

Fire and explosion hazard: Low.

Flash point: (CC) 242°C [51]

(OC) 242°C [51]

uel: unknown

lel: unknown

Autoign. temp.: unknown

Slightly flammable solid. Dangerous. Emits highly toxic fumes of chlorides when heated to decomposition. Fight fire with CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [51],[55]

Incompatibility: Dimethylformamide; strong oxidizing agents. [51],[55]

## 352 - Hexachlorobenzene

**Handling:** Avoid all contact. Keep away from heat and flame. Do not breathe dust, mist, or vapors (appropriate respirator or self-contained breathing apparatus required). Prevent eye and skin contact (chemical resistant gloves, safety goggles, other protective clothing). Use with adequate ventilation (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry secure poison area. [55]

**Health effects:** HCB is a poison and suspected carcinogen. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include lymphatic system, skin, liver, and thyroid gland. It is irritating to mucous membranes and upper respiratory tract. Clinical symptoms include enlargement of the thyroid and lymph nodes, abnormal growth of body hair and weight loss. Reports of death among breast-fed babies are attributed to HCB. Causes photosensitivity. Exposure to light can result in allergic reactions resulting in dermatologic lesions, which can vary from sunburn-like responses to edematous, vesiculated lesions or bullae. Chronic overexposure may cause carcinogenic effects. [56],[55],[75]

**Toxicity:** Moderate.

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: suspected IARC carcinogen [56],[51]

human limited evidence [55]

animal sufficient evidence [55]

Mutagenicity: unknown

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: 220 mg/kg body wt [55]

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown



Hexachlorobutadiene

 $C_4Cl_6$ 

CAS RN: 87-68-3

Syn: Hexachlorobutadiene \* 1,3-Butadiene, 1,1,2,3,4,4-hexachloro- \* C 46 \*  
 Dolen-pur \* GP-40-66:120 \* HCB \* HCBd \* 1,3-Hexachlorobutadiene \*  
 Hexachloro-1,3-butadiene \* Hexachlorobuta-1,3-diene \* 1,1,2,3,4,4-  
 Hexachloro-1,3-butadiene \* Perchlorobutadiene \* RCRA Waste Number U128 \* UN  
 2279 (DOT) \*

Molecular formula:  $CCl_2=CCl-CCl=CCl_2$ 

Polychlorinated Aliphatic Halide

**Physical properties:**

Relative molecular mass:	260.762	
Specific gravity:	1.6820	[51]
	1.675 (15.5/15.5)	[104], [22]
	1.5542 @ 20°C	[105], [106]
Boiling point:	215.°C	[105], [56], [51], [23]
	210.°-220°C	[104], [22]
Melting point:	-21.°C	[105], [51], [106], [23]
	-19.° - -22°C	[104], [22]
Refractive index:	1.5542	[51]
	1.552	[22]
Vapor pressure:	0.020 kPa @ 25°C (0.15mm)	[23]
	2.93 @ 100°C (22mm)	[104]
	66.661 @ 200°C (500mm)	[104]
Vapor density:	8.99	[51]
Evaporation rate:	unknown	
Relative dielectric permittivity:	2.6 @ 20°C	[11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	2.447 mPa-s @ 38°C	[22]
	1.131 @ 99°C	[22]
Kinematic viscosity:	1.479 $\mu m^2/s$ @ 38°C	
	0.724 @ 99°C	
Surface tension:	unknown	
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	unknown	
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	unknown	
Heat of combustion:	unknown	
Heat of formation:	unknown	
Gibbs (free) energy:	unknown	

### 354 - Hexachlorobutadiene

Analytical chemistry:	pP <sub>oct</sub> =	4.9	[23]
		4.78	[4],[31],[41]
		3.74	[8]
	pK <sub>s</sub> =	NA	
	pK <sub>a</sub> =	NA	[31]
	pK <sub>BH</sub> =	NA	
Henry's law constant =		2.6 kPa·m <sup>3</sup> /mol	[41]
		1.04	[41]
		0.103	[41]
Hydrolysis half-life =		NA	[31]

**Electrochemical data:** Meites et al. (1982)

**Clay-organic interaction data:** Unknown

**Solubility:** Almost insoluble in water. Soluble in ethanol, acetone, and ethyl ether. [104],[51],[105]

0.000255 wt% @ 20°C	[23]
0.0002 wt% @ 20°C	[8]

**Form:** Clear, colorless to pale-yellow liquid. Faint turpentine-like odor. [56],[55]

**Use:** Solvent for natural rubber, elastomers, synthetic rubber and other polymers; heat-transfer fluid; transformer liquid; hydraulic fluid; wash liquor for removing C<sub>4</sub> and other higher hydrocarbons; sniffgas recovery agent in chlorine plants; chemical intermediate for fluorinated lubricants and rubber compounds; fluid gyroscopes; fumigant for grapes. [22],[104],[56],[41]

**Fire and explosion hazard:** Very low.

Flash point: None [22]

uel: NA

lel: NA

Autoign. temp.: 610°C [51]

Nonflammable liquid. Emits very toxic fumes of Cl<sup>-</sup>, CO, and CO<sub>2</sub> when heated to decomposition. Fight fire with dry chemical powder, CO<sub>2</sub>, alcohol or polymer foam. [51],[55]

**Incompatibility:** Strong oxidizing agents. [55]

**Handling:** Avoid heat and flame. Do not breathe vapor (appropriate respirator or self-contained breathing apparatus required). Do not get in eyes, on skin, or on clothing (full protective clothing; rubber gloves; goggles and face shield (8-inch minimum)). Avoid any skin contact with this substance. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [56],[51],[55]

**Health effects:** HCB is corrosive and a suspected carcinogen. Routes of entry are ingestion, inhalation, skin absorption, and eye and skin contact. Points of attack include respiratory tract, eyes, skin, liver, and kidneys. It is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. High doses may cause severe kidney injury and cancer. Chronic exposure may damage liver or kidneys and cause cancer. There is a general lack of information concerning the health effects of HCB on humans. [56],[55],[76]

**Toxicity:** High

TWA: 0.02 ppm (0.2 mg/m<sup>3</sup>) (skin) [1]

STEL: unknown

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: 0.56 ppm (0.006 mg/L) [104]

Carcinogenicity: suspected [56],[55]

Mutagenicity: suspected [76]

**Exposure:** Unknown

356 -  $\gamma$ -Hexachlorocyclohexane $\gamma$ -Hexachlorocyclohexane (Lindane) C<sub>6</sub>H<sub>6</sub>Cl<sub>6</sub>

CAS RN: 58-89-9

Syn:  $\gamma$ -Hexachlorocyclohexane \* Cyclohexane, 1,2,3,4,5,6-hexachloro-  
(1 $\alpha$ ,2 $\alpha$ ,3 $\beta$ ,4 $\alpha$ ,5 $\alpha$ ,6 $\beta$ )- \* Cyclohexane, 1,2,3,4,5,6-hexachlori-,  $\gamma$ - \* 666 \*  
 Aalindan \* Aficide \* Agrisol G-20 \* Agroside (2, 7, 6G, III, or WP) \*  
 Agronexit \* Ameisenmittel merck \* Ameisentod \* Aparasin \* Aphitiria \*  
 Aplidal \* Arbitex \* BBH \* Ben-hex \* Bentox 10 \* Benzene hexachloride \*  $\gamma$ -  
 Benzene hexachloride \* Benzene hexachloride-gamma isomer \* Benzene-cis-  
 hexachloride \* Benxol \* BHC \*  $\gamma$ -BHC \* Celanex \* Chloran \* Chloresene \*  
 Codechine \* DBH \* Detmol-extrakt \* Detox 25 \* Devoran \* Dol granule \* Drill  
 tox-spezial aglukon \* ENT 7796 \* Entomoxan \* Exagama \* Fenofort forte \*  
 Forlin \* Forst-nexen \* Gallogama \* Gamacarbattox \* Gamacid \* Gamma-col \*  
 Gamene \* Gammexene \* Gamiso \* *gamma*-Benzene hexachloride \* *gamma*-BHC \*  
*gamma*-HCH \* Gammahexa \* *gamma*-Hexachlor \* *gamma*-Hexachloran \* *gamma*-  
 Hexachlorane \* Gammahexane \* Gammalin \* Gamaphex \* Gammaterre \* Gammex \*  
 Gammexane \* Gammopaz \* Gexane \* HCC \* HCCH \* HCH \*  $\gamma$ -HCH \* Heclotox \* Hexa  
 \* Hexachloran \*  $\gamma$ -hexachloran \* Hexachlorane \*  $\gamma$ -Hexachlorane \*  $\gamma$ -  
 hexachlorobenzene \* 1 $\alpha$ ,2 $\alpha$ ,3 $\beta$ ,4 $\alpha$ ,5 $\alpha$ ,6 $\beta$ -Hexachlorocyclohexane \*  
 Hexachlorocyclohexane gamma-isomer \* 1,2,3,4,5,6-  
 hexachlorocyclohexanegamma-isomer \* Hexatox \* Hexaverm \* Hexicide \*  
 Hexyclan \* HGI \* Hortex \* Hungaria L-7 \*  $\gamma$ -Isomer \* Inexit \* Isotox \*  
 Jacutin \* Kokotine \* Kwell \* Lendine \* Lentox \* Lidenal \* Lindafor \*  
 Lindagam \* Lindagrain \* Lindagranox \* Lindane \*  $\gamma$ -Lindane \* Lindapoudre \*  
 Lindatox \* Lindex \* Lindosep \* Lintox \* Linvur \* Lorexane \* Mglawik L \*  
 Milbol 49 \* Mszycol \* NA 2761 (DOT) \* NCI-C00204 \* Neo-scabacidol \* Nexen  
 FB \* Nexit \* Nexit-stark \* Nexol-E \* Nicochloran \* Novigam \* Omnitox \*  
 Ovadziak \* Owadziak \* Pedraczak \* Pflanzol \* Quellada \* RCRA Waste Number  
 U129 \* Sang-gamma \* Silvanol \* Spritz-Rapidin \* Spruehpflanzol \* Streunex \*  
 TAP 85 \* TBH \* Tri-6 \* Viton \*

Molecular formula: CHClCHClCHClCHClCHClCHCl

Polychlorinated Saturated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	290.832	
Specific gravity:	1.891 @ 19°C	[107]
	1.89	[32]
	1.87	[104], [22]
Boiling point:	323.4°C	[105]
	decomposes >177°C	[32]
Melting point:	113°C	[56]
	112.5°-113°C	[105]
	112.5°C	[108], [22]
	112°C	[104]
Refractive index:	1.644	[108]
Vapor pressure:	1.25x10 <sup>-6</sup> kPa @ 20°C (9.4x10 <sup>-6</sup> mm)	[108]
	4.300x10 <sup>-6</sup> @ 20°C (3.225x10 <sup>-5</sup> )	[41]
	8.9x10 <sup>-6</sup> @ 25°C (6.7x10 <sup>-5</sup> mm)	[41]
Vapor density:	518 ng/l	
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	

Thermal conductivity: unknown  
Electrical resistivity: unknown  
Critical temperature: unknown  
Critical pressure: unknown  
Dynamic viscosity: NA  
Kinematic viscosity: NA  
Surface tension: NA  
Contact angle: NA  
Thermal expansion coefficient: unknown  
Compressibility: NA  
Vapor diffusivity: unknown  
Solution diffusivity: unknown  
Electric dipole moment: unknown  
Ionization potential: unknown  
Magnetic volume susceptibility: unknown  
Speed of sound: unknown  
Heat of melting: unknown  
Heat of vaporization: unknown  
Heat of sublimation: unknown  
Heat capacity @ 25°C: unknown  
Heat of combustion: unknown  
Heat of formation: unknown  
Gibbs (free) energy: unknown

Analytical chemistry:  $pP_{oct}$  = 3.89 [31], [41]  
3.85 [27]  
3.72 [8], [21]  
3.7 [41]  
3.61 [21]  
3.57 [41]  
3.3 [41]  
 $pK_s$  = NA  
 $pK_a$  = NA [31]  
 $pK_{BH}$  = NA  
Henry's law constant = 0.0000248 kPa·m<sup>3</sup>/mol [41]  
0.000329 [41]  
0.0000486 [41]  
Hydrolysis half-life = >1.3x10<sup>8</sup> sec [8]

Electrochemical data: Meites and Zuman (1977)

Clay-organic interaction data: Boucher and Lee (1972), Karickhoff (1981), Lotse et al. (1968), McCall et al. (1980).

Solubility: Almost insoluble in water. Soluble in acetone, benzene, chloroform, ether, ethanol. [108]

17.0 wt% (99% purity) water @ 24°C [104]  
0.001 wt% in water @ 20°C [32]  
0.00078 wt% in water @ 25°C [41]  
43.5 wt% in acetone @ 20°C [108]  
28.9 wt% in benzene @ 20°C [108]  
24.0 wt% in chloroform @ 20°C [108]  
20.8 wt% in ether @ 20°C [108]  
6.4 wt% in ethanol @ 20°C [108]

## 358 - $\gamma$ -Hexachlorocyclohexane

**Form:** Colorless, white, yellowish, or tan to dark brown crystalline solid, powder or solution. Characteristic phosgene-like or musty odor. Pure material is odorless. Technical and commercial mixtures contain one or more of the other stereo-isomers. [108],[22],[56],[32]

**Use:** Insecticide (Lindane) in treatment of animals, buildings, man for ectoparasites, clothes, water for mosquitoes, living plants, seeds, soils; scabicides; pediculicides; vermifuges. Major use recently has been to pretreat seeds. It is toxic to flies, cockroaches, aphids, grasshoppers, wire worms, and boll weevils. [22],[56],[32]

**Fire and explosion hazard:** Very low.

Flash point: NA

UEL: NA

LEL: NA

Autoign. temp.: NA

Non-flammable solid, but may be dissolved in a flammable solvent. When heated to decomposition (>177°C) emits toxic fumes of  $\text{Cl}^-$ ,  $\text{HCl}$ ,  $\text{CO}$ ,  $\text{CO}_2$ , and phosgene. [51],[107],[32]

**Incompatibility:** Alkaline substances; strong oxidizing agents. [22],[55]

**Handling:** Wear protective clothing to avoid any possibility of skin or eye contact (neoprene or polyethylene suit gloves and boots; splash-proof safety goggles). Appropriate respirator or self-contained breathing apparatus required and fully enclosed suit recommended where direct exposure or high concentrations anticipated. Contaminated clothing and shoes should be removed before leaving the work place and not worn until cleaned. Facilities for eye wash and quick body drenching should be available. Keep container tightly closed. Store in cool, dry, secure poison area. [56],[53],[32]

**Health effects:**  $\gamma$ -BHC (commercially known as Lindane) is a poison and possible human carcinogen. Routes of entry are inhalation, skin absorption, ingestion, and eye or skin contact. Points of attack include eyes, central nervous system, blood, liver, kidneys, respiratory system, and skin. Symptoms of acute overexposure include irritation of the eyes, nose and throat, dizziness, headaches, nausea, vomiting, diarrhea, clonic convulsions, respiratory problems, cyanosis, circulatory collapse, aplastic anemia, skin irritations, muscular spasms.  $\gamma$ -BHC is carcinogenic in mice producing liver tumors when administered orally. However, results in rats were considered inadequate. Accidental ingestion in humans has caused fatalities. The effects were repeated, violent, clonic convulsions, sometimes superimposed on a continuous tonic spasm, respiratory difficulty, and cyanosis secondary to the convulsions were common. [56],[108],[32],[79]

**Toxicity:** High.

TWA: 0.04 ppm (0.5 mg/m<sup>3</sup>) (skin) -- for Lindane [1]

STEL: no value set [1]

CL: unknown

IDLH: 84 ppm (1000 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 12.0 mg/kg in water [104]

Carcinogenicity: potential human carcinogen, positive results in some animals [51],[108]

weakly carcinogenic [43]

Mutagenicity: mutagen to human lymphocytes [107]

**Exposure:**

External:

Non-lethal: 111 mg/kg body wt in a child -- systemic effects [51]

Lethal: 180 mg/kg body wt in a child [51]

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: 0.08 ppm (1 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: unknown

Lethal: unknown

## 360 - Hexachloroethane

Hexachloroethane

 $C_2Cl_6$ 

CAS RN: 67-72-1

Syn: Hexachloroethane \* Ethane, hexachloro- \* Avlothane \* Carbon hexachloride \* Distokal \* Distopan \* Distopin \* Egitol \* Ethane hexachloride \* Ethylene hexachloride \* Falkitol \* Fasciolin \* HCE \* 1,1,1,2,2,2-Hexachloroethane \* Hexachloroethylene \* Mottenhexe \* NA 9037 (DOT) \* NCI-C04604 \* Perchlorethane \* Perchloroethane \* Phenohep \* RCRA Waste Number U131 \*

Molecular formula:  $Cl_3C-CCl_3$ 

Polychlorinated Aliphatic Halide

## Physical properties:

Relative molecular mass:	236.7403		
Specific gravity:	2.09		[104], [108]
	2.091	[10], [105], [51], [47], [22]	
	2.1		[32]
Boiling point:	sublimes at melting point		
Melting point:	189.°C	sublimes	[56], [32]
	187.°C	sublimes	[104]
	186.°-187°C	sealed tube	[106], [47], [105]
	186.9°-187.4°C	sealed tube	[10]
	186.6°C	sublimes	[51]
	186.6°-187.4°C		[105]
	186.°C		[105]
	185.°C		[22]
Refractive index:	unknown		
Vapor pressure:	0.0293 kPa	@ 20°C (0.22mm)	[32]
	0.0533	@ 20°C (0.4mm)	[104]
	0.1067	@ 30°C (0.8mm)	[104]
	0.1333	@ 32.7°C (1mm)	[105], [51], [47]
	1.33	@ 73.5°C (10mm)	[105]
Vapor density:	8.16		[104]
Evaporation rate:	unknown		
Relative dielectric permittivity:	unknown		
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	unknown		
Electrical resistivity:	unknown		
Critical temperature:	unknown		
Critical pressure:	unknown		
Dynamic viscosity:	NA		
Kinematic viscosity:	NA		
Surface tension:	NA		
Contact angle:	NA		
Thermal expansion coefficient:	unknown		
Compressibility:	NA		
Vapor diffusivity:	unknown		
Solution diffusivity:	unknown		
Electric dipole moment:	unknown		
Ionization potential:	unknown		
Magnetic volume susceptibility:	-12.5x10 <sup>-6</sup> SI units	@ 20°C	[105]
Speed of sound:	unknown		
Heat of melting:	9.755 kJ/mol		[10]



Heat of vaporization:	49.0329 kJ/mol	[105]
	51.079	[10]
Heat of sublimation:	51.08 kJ/mol	[108]
	69.08 @ 25°C	[10]
Heat capacity @ 25°C:	0.1368 (gas)	[10]
Heat of combustion:	580.7 kJ/mol @ 25°C (sol)	[20]
	639.7 (gas)	[20]
	460.55 @ 20°C (sol)	[105]
Heat of formation:	-206.8 kJ/mol @ 25°C (sol)	[20]
	-192.6 (sol)	[105]
	-139.00 (gas)	[10]
	-147.8 (gas)	[20]
Gibbs (free) energy:	-54.97 kJ/mol @ 25°C (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	4.62	[31],[41]
	3.93	[27],[41]
	3.82	[23]
	3.58	[41]
	3.34	[8]
	pK <sub>s</sub> =	NA
	pK <sub>a</sub> =	NA [31]
	pK <sub>BH</sub> =	NA
Henry's law constant =	221. kPa-m <sup>3</sup> /mol @ 25°C	[41]
Hydrolysis half-life =	NA	[31]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Almost insoluble in water. Soluble in, benzene, chloroform, oils. Very soluble in ethanol, ether. [51],[47],[104],[10]  
 0.005 wt% water @ 20°C [104]  
 0.005 wt% water @ 22°C [104],[10],[47]

Form: Colorless rhombic, triclinic or cubic crystals. Camphor-like odor. Readily sublimates without melting. [51],[108],[56]

Use: Manufacture of smoke candles and grenades; by-product of industrial chlorination process; plasticizer for cellulose esters; minor use in rubber and insecticidal formulations; medicinal manufacturing; anthelmintic to treat fascioliasis in sheep and cattle; moth repellent; retardant in fermentation process in feed for ruminants; fire extinguishing fluids manufacturing; camphor substitute in cellulose solvent; refining aluminum alloys; removing impurities from molten metals; recovering metals from ores or smelting products; improving quality of various metals and alloys. [104],[56]

Fire and explosion hazard: Very low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

## 362 - Hexachloroethane

Nonflammable solid. Explosion hazard is slight, but dehalogenation by reaction with alkalis, metals, etc. will produce spontaneously explosive chloroacetylenes. Emits highly toxic fumes (such as phosgene, chlorine, carbon tetrachloride, tetrachloroethylene, carbon monoxide and carbon dioxide) when heated to decomposition. [51],[32],[55]

**Incompatibility:** Alkalies; zinc; aluminum; hot iron; strong oxidizing agents; strong bases. [32],[56],[55]

**Handling:** Avoid heat and flame. Prevent inhalation of vapor, mist, or dust (appropriate respirator or self-contained breathing apparatus). Prevent repeated or prolonged skin or eye contact (chemical resistant gloves; safety goggles; protective overclothing). Wash promptly when skin is wet or contaminated and daily at the end of each work shift. Work clothing should be changed daily if it is possible that clothing is contaminated. Remove nonimpervious clothing promptly if contaminated. Discard contaminated clothing and shoes. Provide emergency showers and eye wash stations. Keep container tightly closed. Store in a cool, dry, secure poison area. [56],[55]

**Health effects:** Hexachloroethane is a toxin and potential carcinogen. Routes of entry are inhalation, skin absorption, ingestion, and eye and skin contact. Points of attack include eyes, central nervous system, upper respiratory system, and liver. It acts primarily as a central nervous system depressant, and in high concentrations it causes narcosis. It is also moderately irritating to the skin, mucous membranes and liver. Exposure to the hot fumes may cause irritation to the eyes. No chronic effects have been reported from industrial exposure, although significant absorption through the skin can occur. Low vapor pressure of this compound as well as its solid state minimize its inhalation hazards. [32],[56],[55]

**Toxicity:** Very high.

TWA: 10 ppm (100 mg/m<sup>3</sup>) intended to be changed to 1 ppm (10 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: 300 ppm (2900 mg/m<sup>3</sup>) [56]

Peak: unknown

Odor threshold: 0.010 mg/kg in water [104]

Carcinogenicity: positive in mice and negative in rats [51],[56],[40]

Mutagenicity: unknown

**Exposure:** Unknown

## Hydrogen Cyanide

HCN

CAS RN: 74-90-8

Syn: Hydrogen cyanide \* Hydrocyanic acid \* Carbon hydride nitride \*  
 Evercyn \* Formic anammonide \* Formonitrile \* Prussic acid \*

Molecular formula: HCN

Cyanide

## Physical properties:

Relative molecular mass:	27.03	
Specific gravity:	0.688 (liq)	[22],[107],[10],[51]
	0.6876	[105]
	0.938 g/L (gas)	[22]
	0.941 (gas)	[108]
Boiling point:	25.6°C	[22],[104],[108]
	25.7°C	[107],[51],[10],[106],[16],[105]
Melting point:	-13.2°C	[51],[106],[16],[105]
	-13.3°C	[22],[107],[104],[10]
	-13.4°C	[105],[108]
Refractive index:	1.2614	[106],[16],[105]
Vapor pressure:	0.133 kPa @ -71.0°C (1mm)	[105],[20]
	1.333 @ -47.7°C (10mm)	[105],[20]
	5.333 @ -30.9°C (40mm)	[105],[20]
	13.332 @ -17.8°C (100mm)	[105],[20]
	53.33 @ 10.2°C (400mm)	[105],[20]
	82.6 @ 20°C (620mm)	[104]
	101.32 @ 25.9°C (760mm)	[105],[20]
Vapor density:	0.94	[104]
	0.932	[51]
Evaporation rate:	unknown	
Relative dielectric permittivity:	114.9 @ 20°C	[105],[11],[7]
	116. @ 20°C	[10]
	152. @ 0°C	[11]
	107. @ 25°C	[11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.0671 W/(m-K) @ 15.6°C	[105]
Electrical resistivity:	3.03x10 <sup>-3</sup> MOhm-m @ 0°C	[10],[11]
	22.2x10 <sup>-3</sup> @ 18°C	[11]
Critical temperature:	183.5°C	[10],[105],[107],[20],[47]
Critical pressure:	4.95 MPa	[105]
	5.39	[10],[20],[47]
Dynamic viscosity:	0.206 mPa-s @ 18°C	[10]
Kinematic viscosity:	0.296 μm <sup>2</sup> /s @ 18°C	
Surface tension:	19.45 mN/m @ 10°C	[10]
	18.33 @ 20°C	[10],[7]
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	17.3 μm <sup>2</sup> /s @ 0°C in air	[47],[59]
Solution diffusivity:	1.7 nm <sup>2</sup> /s (calc)	[59]
Electric dipole moment:	9.94x10 <sup>-30</sup> C-m	[105],[10]
Ionization potential:	13.8 eV (EI)	[105]
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	

### 364 - Hydrogen Cyanide

Heat of melting:	8.418 kJ/mol	[107]
	8.412	[105]
	8.411	[10],[20]
Heat of vaporization:	30.726 kJ/mol	[105]
	25.23	[10]
	27.9	[7]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.071 kJ/(mol-K) (liq)	[105],[10]
	0.036 (gas)	[105],[10]
Heat of combustion:	-645.73 kJ/mol @ 25°C (liq)	[20]
	-672.0 (gas)	[20]
Heat of formation:	130.6 @ 25°C (gas)	[7]
	108.9 (liq)	[10],[20],[105]
	135.2 (gas)	[10],[20],[105]
Gibbs (free) energy:	125.0 @ 25°C (liq)	[10],[105]
	125. (gas)	[10],[105]
Analytical chemistry: pP <sub>oct</sub> =	0.66	[68]
	0.35	[104]
	1.07 (calculated)	[104]
pK <sub>s</sub> =	unknown	
pK <sub>a</sub> =	9.31 in water @ 25°C	[105]
	9.21 in water @ 25°C	[10]
pK <sub>BH</sub> =	unknown	
Henry's law constant =	unknown	
Hydrolysis half-life =	unknown	

Electrochemical data: Unknown

Clay-organic interaction data: [8]

Solubility: Soluble in ether. Miscible with water, alcohol. [105],[22],[10],[47]

Form: Water-white to colorless liquid at temperatures below 26.5°C. Faint odor of bitter almonds. A very weak acid. Commercial material is 96-99.5% pure. Sensitive to light. The liquid is commonly stabilized by addition of acids. [22],[107],[108],[51]

Use: Manufacture of acrylonitrile, acrylates, adiponitrile, cyanide salts, dyes; chelates; electroplating; steel hardening; gold and silver extraction from ores; fumigating. [22],[56]

Fire and explosion hazard: Very high.

Flash point: (CC) -17.8°C [107],[51]

uel: 40.0% [107],[51]

lel: 5.6% [107],[51]

Autoign. temp.: 538°C [22],[51]

540°C [107]

Highly flammable gas or liquid. It is very explosive. A very dangerous fire hazard when exposed to heat, flame, or oxidizers. Can polymerize at 50°-60°C, or catalyze with traces of alkali, explosively. Burns in air with a blue flame. Fight fire with CO<sub>2</sub>, non-alkaline dry chemical powder, alcohol or polymer foam. Do not use water. [22],[51],[107]

**Incompatibility:** Bases such as caustics; amines. Can react violently with acetaldehyde. [56],[51]

**Handling:** Avoid heat, flame, sparks, or other sources of ignition. Prevent any possibility of inhalation of mist, vapor, or fumes (self-contained breathing apparatus required). Prevent any contact with skin, eyes, or clothing (chemical protective suit; gloves; face shield). Wash immediately if skin is contaminated and remove clothing to avoid flammability hazard. Provide quick-opening safety showers and eyewash stations. Store in secure poison area. Store in cool, dry, well-ventilated, flammable liquid storage area. [107],[56]

**Health effects:** Hydrogen cyanide is highly toxic and an asphyxiant. Routes of entry are ingestion, inhalation, and skin and eye contact. Points of attack include the respiratory system, liver, kidneys, cardiovascular system, and central nervous system. Symptoms of overexposure are irritation of throat, palpitation, difficult breathing, reddening of eyes, salivation, nausea, headache, weakness of arms and legs, giddiness which can be followed by collapse, convulsions, unconsciousness, and death. Human deaths from ingestion, inhalation, and injection have been recorded. [22],[107],[56],[51],[32],[68]

**Toxicity: High**

TWA: no value set [1]  
 STEL: no value set [1]  
 CL: 10 ppm (11 mg/m<sup>3</sup>) (skin) [1]  
 IDLH: 50 ppm (55 mg/m<sup>3</sup>) [107]  
 Peak: unknown  
 Odor threshold: 1 ppm (1 mg/m<sup>3</sup>) [107]  
 Carcinogenicity: unknown  
 Mutagenicity: indefinite [68]

**Exposure:**

**External:**

Non-lethal: unknown  
 Lethal: 1 mg/kg body wt -- death of an adult human by injection [51]

**Oral:**

Non-lethal: unknown  
 Lethal: 0.57 mg/kg body wt -- death of an adult human [51]  
 1.47 mg/kg body wt -- death of an adult male [51]

**Inhalation:**

Short-term Inhalation Limits: 20 ppm (22 mg/m<sup>3</sup>) for 30 min [107]  
 Non-lethal: 20 ppm (22 mg/m<sup>3</sup>) -- symptoms of illness [104]  
 40 ppm (44 mg/m<sup>3</sup>) -- severe effects [104]  
 Lethal: 110 ppm (120 mg/m<sup>3</sup>) -- can be fatal in 1 hr [32],[51]  
 135 ppm (150 mg/m<sup>3</sup>) -- fatal with 30 min exposure [104]  
 181 ppm (200 mg/m<sup>3</sup>) -- death of an adult human in 10 min  
 [32],[104],[51]  
 270 ppm (300 mg/m<sup>3</sup>) -- death of an adult human instantly  
 [32],[104],[51]

## 366 - Isophorone

Isophorone

C<sub>9</sub>H<sub>14</sub>O

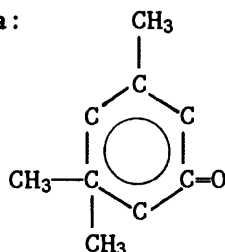
CAS RN: 78-59-1

Syn: Isophorone \* 2-Cyclohexen-1-one, 3,5,5-trimethyl- \* Isoacetophorone \* Isoforon \* Isooctaphenone \* α-Isophoron \* Isophorone \* α-Isophorone \* NCI-C55618 \* 1,1,3-trimethyl-3-cyclohexene-5-one \* 3,5,5-Trimethyl-5-cyclohexen-1-one \* 3,5,5-Trimethyl-2-cyclohexene-1-one \* Trimethylcyclohexenone \* UN 1224 (DOT) \*

Molecular formula: COCH=C(CH<sub>3</sub>)CH<sub>2</sub>C(CH<sub>3</sub>)<sub>2</sub>CH<sub>2</sub>

Cyclic Ketone

Structural formula:



## Physical properties:

Relative molecular mass:	138.21	
Specific gravity:	0.92	[104]
	0.9229	[105], [51], [106]
	0.921 @ 25°C	[107]
Boiling point:	215.3°C	[107]
	215.2°C	[10], [51], [22]
	215.°C	[56], [104]
	214.°C	[105]
Melting point:	-8.°C	[104]
	-8.1°C	[10], [107], [22]
Refractive index:	1.4759	[10], [105], [106]
Vapor pressure:	0.0267 kPa @ 20°C (0.2mm)	[22]
	0.0507 @ 20°C (0.38mm)	[104]
	0.1333 @ 38°C (1mm)	[105], [51]
	1.333 @ 81.2°C (10mm)	
Vapor density:	4.77	[51], [104]
	4.75	[107]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	2.62 mPa·s @ 20°C	[22]
Kinematic viscosity:	2.83 μm <sup>2</sup> /s @ 20°C	
Surface tension:	32.3 mN/m @ 20°C	[107]
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	



### 368 - Isophorone

**Handling:** Keep away from heat and open flame. Prevent inhalation of mist or vapors (appropriate respirator or self-contained breathing apparatus). Prevent any possibility of skin or eye contact (rubber gloves; protective overclothing; splash-proof chemical goggles or face shield). Wash promptly if skin is wet or contaminated. Use with good ventilation (fume hood). Provide emergency shower and eyewash stations. Keep container tightly closed. Store in a cool, dry, secure poison area. [56],[57],[55]

**Health effects:** Isophorone is an irritant and poison. Routes of entry are inhalation, ingestion, and eye and skin contact. Points of attack include kidneys, respiratory system, and skin. It is chiefly a kidney poison. It can cause irritation of eyes, nose, and throat, narcosis, dermatitis, headaches, dizziness, lachrymation, possible opacity of the cornea and necrosis of the cornea. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Ingestion causes irritation of mouth and stomach. Liquid or solid may cause smarting of the skin and first-degree burns on short exposure and may cause second degree burns on long exposure. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. [51],[56],[107],[55]

**Toxicity:** Low.

TWA: no value set [1]

STEL: no value set [1]

CL: 5 ppm (15 mg/m<sup>3</sup>) [1],[56]

IDLH: 800 ppm (4500 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 0.20-0.54 ppm (1.13-3.05 mg/m<sup>3</sup>) [104]

Carcinogenicity: inconclusive results in small animals [26]

Mutagenicity: no genotoxicity found [44]

significant response in tests [37]

**Exposure:**

External:

Non-lethal: 25 ppm (140 mg/m<sup>3</sup>) for 15 min -- may be irritating to eyes, nose, and throat [51],[104]

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown



Lead

Pb

CAS RN: 7439-92-1

Syn: Lead \* Pb \* C.I. 77575 \* C.I. Pigment metal 4 \* Glover \* KS-4 \* Lead  
flake \* Lead S2 \* Lead S0 \* Omaha \* Omaha & Grant \* S0 \* S1 \*

Molecular formula: Pb

Element

## Physical properties:

Relative molecular mass:	207.2	
Specific gravity:	11.34	[10],[51],[108],[48]
	11.35	[22],[105]
Boiling point:	1620.°C	[47]
	1730.°C	[48]
	1740.°C	[51],[105],[108]
	1753.°C	[10]
	1755.°C	[22]
Melting point:	327.3°C	[48]
	327.4°C	[108],[22]
	327.43°C	[51]
	327.5°C	[10],[47]
	327.502°C	[105]
Refractive index:	2.01	[105]
	2.6	[105]
Vapor pressure:	0.133 kPa @ 970°C (1mm)	[105]
	0.133 @ 973°C (1mm)	[47],[51]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	NA	
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	35.123 W/(m-K) @ 0°C	[48]
	35.6 @ 0°C	[105]
	34.62 @ 18°C	[10]
	34.774 @ 20°C	[48]
	35.3 @ 25°C	[105]
	34.6 @ 25°C	[105]
Electrical resistivity:	2.065x10 <sup>-13</sup> MOhm-m @ 20°C	[108]
	2.1x10 <sup>-13</sup> @ 22°C	[105]
	2.702x10 <sup>-13</sup> @ 100°C	[108]
Critical temperature:	5126.8 °C	[20]
Critical pressure:	8388.8 MPa	[20]
Dynamic viscosity:	2.58 mPa-s @ 350°C	[105]
Kinematic viscosity:	0.0125 µm <sup>2</sup> /s @ 350°C	
Surface tension:	453. mN/m @ 350°C	[20]
	452. @ 360°C	[105]
	423. @ 750°C	[20]
Contact angle:	NA	
Thermal expansion coefficient:	0.000029 K <sup>-1</sup> @ 20°C	[48]
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	NA	
Ionization potential:	7.415 eV (VUS)	[105]
Magnetic volume susceptibility:	-289.0x10 <sup>-6</sup> (sol) SI units @ 15.8 °C	[105]

### 370 - Lead

	-194.7x10 <sup>-6</sup> (liq) SI units @ 56.8°C	[105]
Speed of sound:	2160. m/s long.wave in bulk annealed	[105]
	1960. long. wave in bulk rolled	[105]
	1190. long.wave in thin rod annealed	[105]
	700. shear wave in bulk annealed	[105]
	690. shear wave in bulk rolled	[105]
	1210. long. wave in thin rod rolled	[105]
Heat of melting:	4.78 kJ/mol	[10]
	4.94	[48]
	5.12	[105],[47]
Heat of vaporization:	176.1 kJ/mol	[47]
	178.1	[10]
	178.7	[108]
	190.9	[48]
Heat of sublimation:	195.7 kJ/mol	[10]
Heat capacity @ 25°C:	0.0268 kJ/(mol-K) (sol)	[10]
	0.0267 (liq-Pb <sup>2+</sup> )	[105]
	0.0268 (liq)	[10]
	0.0208 (gas)	[10]
Heat of combustion:	unknown	
Heat of formation:	0. kJ/mol @ 25°C (sol)	[105],[10]
	1.63 (liq-Pb <sup>2+</sup> )	[105]
	4.291 (liq)	[10]
	194.0 (gas)	[105]
	195.7 (gas)	[10]
Gibbs (free) energy:	0. kJ/mol @ 25°C (sol)	[105],[10]
	-24.3 (liq-Pb <sup>2+</sup> )	[105]
	2.223 (liq)	[10]
	161.1 (gas)	[105]
	162.7 (gas)	[10]
Analytical chemistry:	pP <sub>oct</sub> = NA	
	pK <sub>s</sub> = NA	
	pK <sub>a</sub> = 7.8 (Pb <sup>2+</sup> )	[10]
	pK <sub>BH</sub> = NA	
	Henry's law constant = NA	
	Hydrolysis half-life = NA	

**Electrochemical data:** Sharpe (1973)

**Clay-organic interaction data:** inorganic

**Solubility:** Insoluble in hot and cold water, but dissolves slowly in water containing a weak acid. Soluble in HNO<sub>3</sub>, highly concentrated H<sub>2</sub>SO<sub>4</sub>.  
[22],[105],[47]

**Form:** Bluish-gray, bright luster, highly malleable, ductile, soft metal. Cubic crystal structure. It is a poor conductor of electricity, relatively impenetrable to radiation, good sound and vibration absorber, and very resistant to corrosion. Tarnishes upon exposure to air. It has atomic number 82 (Group IVA) and valence states of +2 and +4. There are 4 stable isotopes. [105],[51],[108],[22]

**Use:** Construction material for tank linings, piping, and other equipment handling corrosive gases and liquids used in the manufacture of sulfuric acid, petroleum refining, halogenation, sulfonation, extraction, condensation; for x-ray and atomic radiation protection; manufacture of tetraethyl lead, pigments for paints, and other organic and inorganic lead compounds; bearing metal and alloys; storage batteries; in ceramics, plastics, and electronic devices; in building construction; in solder and other lead alloys; in the metallurgy of steel and other metals. [108]

**Fire and explosion hazard:** Low.

Flash point: NA

UEL: NA

LEL: NA

Autoign. temp.: NA

Noncombustible solid. Moderate fire and explosion hazard in the form of dust when exposed to heat or flame. Emits highly toxic fumes when heated. Can react vigorously with oxidizing materials. Use extinguishing media appropriate to surrounding fire conditions. [51],[22],[55]

**Incompatibility:** Oxidants; active metals like sodium, potassium; strong acids. **WARNING:** violent reactions of lead with ammonium nitrate, hydrogen peroxide, sodium azide, zirconium, sodium acetylide and chlorine trifluoride have been reported. [51],[55]

**Handling:** Do not breathe dust, vapor, or mist (appropriate respirator or self-contained breathing apparatus). Prevent repeated or prolonged skin contact (leather gloves and suit; safety goggles or face shield). Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Wash daily at the end of each work shift. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [56],[57]

**Health effects:** Lead can be highly toxic. Routes of entry are inhalation, ingestion, and skin absorption. Points of attack include central nervous system, gastrointestinal system, blood, and kidneys. It is irritating to mucous membranes and upper respiratory tract. Symptoms of lead poisoning are decreased physical fitness, fatigue, sleep disturbance, headache, aching bones and muscles, digestive symptoms (particularly constipation), abdominal pains, and decreased appetite. These symptoms are reversible and complete recovery is possible. Later symptoms may include anemia, pallor, a "lead line" on the gums, and decreased hand-grip strength. Lead colic produces an intense periodic abdominal cramping associated with severe constipation and, occasionally, nausea and vomiting. Ingestion or inhalation of large amounts of lead usually affect the central nervous system and may result in severe headache, convulsions, coma, delirium, and possible death. The kidneys can also be damaged after long periods of exposure to lead, with loss of kidney function and progressive azotemia. Content of blood  $>0.05$  mg% and of urine  $>0.08$  mg per liter support a diagnosis of lead poisoning. FDA regulations require zero lead content in foods and 0.05% in house paints. [108],[22],[107],[78]

## 372 - Lead

### Toxicity: High.

TWA: 0.02 ppm (0.15 mg/m<sup>3</sup>) (as dust and fumes) [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: indefinite [51]

animal inadequate evidence (IARC cancer review) [55]

probable [78]

Mutagenicity: experimental teratogen [51]

### Exposure:

#### External:

Non-lethal: unknown

Lethal: unknown

#### Oral:

Non-lethal: 450 mg/kg/6 years -- CNS effects in an adult female [51]

Lethal: unknown

#### Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown

## Mercury

Hg

CAS RN: 7439-97-6

Syn: Mercury \* Hg \* Colloidal mercury \* Metallic mercury \* NA 2809 (DOT) \*  
 NCI-C60399 \* Quicksilver \* RCRA Waste Number U151 \* UN 2809 (DOT) \*

Molecular formula: Hg

Element

## Physical properties:

Relative molecular mass:	200.59	
Specific gravity:	13.5	[32]
	13.5457	[10], [48]
	13.546	[47], [51]
	13.5464	[16]
	13.55	[107]
	13.59	[22]
	13.5939	[105]
Boiling point:	356.-357°C	[107]
	356.58°C	[105]
	356.6°C	[10], [22]
	356.706°C	[16]
	356.72°C	[108]
	356.9°C	[51], [47]
	356.95°C	[48]
	357.°C	[32], [107]
Melting point:	-36.87°C	[16]
	-38.83°C	[48]
	-38.85°C	[22]
	-38.86°C	[10]
	-38.87°C	[47], [105], [108]
	-38.89°C	[51]
	-38.9°C	[107]
	-39.°C	[32]
Refractive index:	1.6-1.9	[105]
Vapor pressure:	2.6x10 <sup>-4</sup> kPa @ 20°C (0.0012mm)	[32]
	2.45x10 <sup>-4</sup> @ 25°C (0.00184mm)	[16]
	2.7x10 <sup>-4</sup> @ 25°C (0.002mm)	[51], [108]
	0.133 @ 126.2°C (1mm)	[47], [51]
Vapor density:	unknown	
Evaporation rate:	unknown	
Relative dielectric permittivity:	1.00074 @ 180°C	[105]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	7.82 W/(m-K) @ 0°C	[105]
	8.141-10.467 @ 0°C	[48]
	10.38 @ 0°C	[10]
	9.304 @ 20°C	[48]
	8.30 @ 25°C	[105]
	8.39 @ 25°C	[105]
Electrical resistivity:	9.41x10 <sup>-13</sup> MOhm-m @ 0°C	[10], [11]
	9.576x10 <sup>-13</sup> @ 20°C	[108]
	9.84x10 <sup>-13</sup> @ 50°C	[105]

### 374 - Mercury

Critical temperature:	900.°C	[10]	
	1460.°C	[48]	
	1462.°C	[107]	
	>1550.°C	[47]	
Critical pressure:	18.24 MPa	[10]	
	>20.3	[47]	
	105.6	[48]	
	160.8	[107]	
Dynamic viscosity:	1.764 mPa-s @ -10°C	[105], [48]	
	1.685 @ 0°C	[105], [48]	
	1.615 @ 10°C	[105], [48]	
	1.56 @ 19.02°C	[105]	
	1.554 @ 20°C	[105], [48]	
	1.55 @ 20.2°C	[105]	
	1.499 @ 30°C	[105], [48]	
Kinematic viscosity:	0.130 μm²/s @ -10°C		
	0.124 @ 0°C		
	0.119 @ 10°C		
	0.12 @ 19.02°C		
	0.115 @ 20°C		
	0.114 @ 20.2°C		
	0.111 @ 30°C		
Surface tension:	480.3 mN/m @ 0°C	[20]	
	487. @ 15°C	[20]	
	470. @ 19°C	[20]	
	470. @ 20°C	[107]	
	484. @ 25°C	[108]	
	467.1 @ 60°C	[20]	
Contact angle:	[18]		
	sessile	advancing	receding
quartz	136	NA	NA
calcite	136	NA	NA
biotite	138	NA	NA
Ca-mont.	158	NA	NA
Thermal expansion coefficient:	0.0001819 K <sup>-1</sup> @ 10°C	[48]	
	0.0001820 @ 20°C	[48]	
	0.0001820 @ 30°C	[48]	
Compressibility:	0.040 nPa <sup>-1</sup> @ 0°C	[105]	
	0.040 @ 20°C	[105]	
	0.041 @ 40°C	[105]	
Vapor diffusivity:	11.2 μm²/s @ 0°C	[47]	
Solution diffusivity:	unknown		
Electric dipole moment:	NA		
Ionization potential:	10.43 eV (VUS)	[105]	
Magnetic volume susceptibility:	-420.2x10 <sup>-6</sup> SI units @ 19.8°C	[105]	
Speed of sound:	1450. m/s @ 25°C	[105]	
Heat of melting:	2.33 kJ/mol	[105], [47]	
	2.27	[107]	
	2.297	[10]	
	2.35	[48]	

Heat of vaporization:	58.53 kJ/mol	[47]
	59.16	[10]
	59.30	[16]
	60.47	[48]
	61.34	[108]
Heat of sublimation:	61.34 kJ/mol	[10]
Heat capacity @ 25°C:	0.0279 kJ/(mol-K) (liq)	[105]
	0.02800 (liq)	[10], [108]
	0.02080 (gas)	[10]
Heat of combustion:	unknown	
Heat of formation:	0. kJ/mol @ 25°C (liq)	[105], [10]
	60.88 (gas)	[105]
	61.36 (gas)	[10]
Gibbs (free) energy:	0. kJ/mol @ 25°C (liq)	[105], [10]
	31.78 (gas)	[105]
	31.87 (gas)	[10]
Analytical chemistry:	pP <sub>oct</sub> =	NA
	pK <sub>s</sub> =	NA
	pK <sub>a</sub> =	3.55 (Hg <sup>2+</sup> ) [10]
	pK <sub>BH</sub> =	NA
	Henry's law constant =	NA
	Hydrolysis half-life =	NA

Electrochemical data: Wrona and Galus (1982)

Clay-organic interaction data: inorganic

Solubility: Almost insoluble in hot and cold water, ethanol, ether, sulfuric acid, and dilute HCl, HBr, HI or cold H<sub>2</sub>SO<sub>4</sub>. Slightly soluble in water in presence of nitrates, ammonium salts, HNO<sub>3</sub>, carbon dioxide. [22], [47], [105], [56]

0.002 wt% water @ 20°C [32]

Form: Silvery-white, heavy, metallic liquid. The only common metal liquid at ordinary temperatures. A relatively poor conductor of heat and a fair conductor of electricity. Solid mercury is a tin-white, ductile, malleable mass which may be cut with a knife. It has atomic number 80 (Group IIB) with valence states of +1 or +2. There are 4 stable isotopes and 12 artificially radioactive isotopes. It rarely occurs free in nature. The chief ore is cinnabar (HgS). [105], [51], [108], [22]

Use: In barometers, thermometers, hydrometers, pyrometers; in mercury arc lamps producing ultraviolet rays; in switches, fluorescent lamps; in mercury boilers; manufacture all mercury salts, mirrors; as catalyst in oxidation of organic compounds; extracting gold and silver from ores; making amalgams, electric rectifiers, mercury fulminate; also in dentistry; in determining N by Kjeldahl method, for Millon's reagent; as cathode in electrolysis, electroanalysis, and many other uses; in pharmaceuticals; agricultural chemicals; antifouling paints. [108]

### 376 - Mercury

**Fire and explosion hazard:** Very low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable. Use extinguishing media appropriate to surrounding fire conditions. [55]

**Incompatibility:** Acetylenic compounds; boron diiodophosphide; ethylene oxide; metals; methylsilane; oxygen; oxidants; tetracarbonylnickel;  $\text{NH}_3$ ;  $\text{BPI}_2$ ;  $\text{Cl}_2$ ;  $\text{CH}_3\text{N}_3$ ;  $\text{Na}_2\text{C}_2$ ; nitromethane; (butyne diol + acid). **WARNING:** mixtures of mercury with acetylene, ammonia, chlorine dioxide, methyl azide, chlorates, nitrates, and hot sulfuric acid can be explosive. [51],[107],[22],[32],[55]

**Handling:** **WARNING:** handle with extreme care. Do not breathe vapor, mist or fumes (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (rubber gloves and suit; safety goggles or face shield; protective overclothing). Readily absorbed through skin, respiratory system, and gastrointestinal tract. Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Work clothing should be changed daily if possibly contaminated. Remove nonimpervious clothing promptly if wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a secure poison area or cabinet. [55],[56],[57]

**Health effects:** Mercury is highly toxic. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include skin, respiratory system, central nervous system, kidneys, and eyes. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Inhalation of vapor may cause headaches, cough, chest pains, chest tightness, and difficulty in breathing. Liquid mercury may irritate the skin. Repeated or prolonged exposure to mercury liquid or vapor can cause fine shaking of the hands, eyelids, lips, tongue, or jaw. Other effects include allergic skin rash, chemical pneumonitis, soreness of the mouth, nausea, diarrhea, loose teeth, insomnia, excess salivation, personality change, irritability, indecision, loss of memory, and intellectual deterioration. Known to adversely affect the fetus if the mother is exposed during pregnancy. The FDA permits zero addition to the 20 micrograms of mercury contained in the average diet. [22],[32],[55],[80]

**Toxicity:** High.

TWA: 0.0012 ppm (0.01 mg/m<sup>3</sup>) (skin) -- alkyl compounds [1]

0.006 ppm (0.05 mg/m<sup>3</sup>) (skin) -- all forms except alkyl vapor [1]

0.012 ppm (0.1 mg/m<sup>3</sup>) (skin) -- aryl and inorganic compounds [1]

STEL: 0.004 ppm (0.03 mg/m<sup>3</sup>) (skin) -- alkyl compounds [1]

CL: 0.012 ppm (0.1 mg/m<sup>3</sup>) [51],[56]

IDLH: 3.4 ppm (28 mg/m<sup>3</sup>) [56],[107]

Peak: unknown

Odor threshold: odorless [32],[107]

Carcinogenicity: noncarcinogenic [80]

Mutagenicity: experimental equivocal tumorigenic agent [51]



Exposure:

External: unknown

Non-lethal: unknown

Lethal: unknown

Oral: unknown

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: 0.018 ppm (150  $\mu\text{g}/\text{m}^3$ ) for 46 days -- gastrointestinal and  
CNS effects in an adult female [51]

0.15-1.03 ppm (1.2-8.5  $\text{mg}/\text{m}^3$ ) -- cough, chest pain, and  
dyspnea [32]

Lethal: unknown

## 378 - Methanol

Methanol

CH<sub>4</sub>O

CAS RN: 67-56-1

Syn: Methanol \* Carbinol \* Colonial spirit \* Columbian spirits \* Methyl alcohol \* Methyl hydrate \* Methyl hydroxide \* Methylol \* Monohydroxymethane \* Pyroxylic spirit \* RCRA Waste Number U154 \* UN 1230 (DOT) \* Wood alcohol \* Wood naphtha \* Wood spirit \*

Molecular formula: CH<sub>3</sub>OH

Aliphatic Alcohol

## Physical properties:

Relative molecular mass:	32.04216	
Specific gravity:	0.79104	[49]
	0.7913	[10]
	0.7914	[105], [106]
	0.7915	[51], [108]
	0.792	[47], [107], [48]
	0.7924	[22]
	0.8	[32]
Boiling point:	65.°C	[106], [104]
	64.97°C	[105]
	64.8°C	[51]
	64.7°C	[47], [10], [108]
	64.546°C	[49]
	64.51°C	[48]
	64.5°C	[107], [32], [22]
	64.°-65°C	[56]
Melting point:	-93.9°C	[105], [106]
	-97. - -98°C	[47]
	-97.7°C	[10]
	-97.68°C	[49]
	-97.8°C	[51], [108], [107], [22]
	-98.°C	[32], [104], [48]
Refractive index:	1.32840	[49]
	1.3288	[105], [106]
	1.329	[22]
	1.3292	[108]
	1.3284 @ 20°C	[10]
Vapor pressure:	0.667 kPa @ -25.3°C (5mm)	[47]
	0.133 @ -16.2°C (10mm)	[105], [47]
	2.67 @ -6.0°C (20mm)	[47]
	5.33 @ 5.0°C (40mm)	[105], [47]
	8.00 @ 12.1°C (60mm)	[47]
	12.27 @ 20°C (92mm)	[104], [22]
	13. @ 20°C (97mm)	[32]
	13.33 @ 21.2°C (100mm)	[51], [105]
	16.937 @ 25°C (127.04mm)	[49]
	21.33 @ 30°C (160mm)	[104]
	26.66 @ 34.8°C (200mm)	[47]
	53.32 @ 49.9°C (400mm)	[105]
Vapor density:	1.1	[107], [104]
	1.11	[108], [51], [32]
Evaporation rate:	2.10	[49]
	4.6	[3]
	5.9	[32]

Relative dielectric permittivity:	40.	@ -20°C	[105],[11]
	37.98	@ 0°C	[10],[20]
	35.5	@ 10°C	[2]
	34.86	@ 15°C	[2]
	33.64	@ 20°C	[10],[20]
	33.62	@ 20°C	[11]
	33.38	@ 20°C	[2]
	33.00	@ 25°C	[2]
	32.63	@ 25°C	[105],[11]
	32.66	@ 25°C	[49]
	32.70	@ 25°C	[10]
	31.38	@ 30°C	[2]
	31.19	@ 35°C	[2]
	29.73	@ 40°C	[20]
	29.05	@ 40°C	[2]
	27.03	@ 50°C	[2]
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	0.216	W/(m-K) @ -20°C	[20]
	0.214	@ 0°C	[48]
	0.210	@ 0°C	[20]
	0.207	@ 12°C	[10]
	0.212	@ 20°C	[48]
	0.2023	@ 20°C	[105]
	0.204	@ 20°C	[20]
	0.212	@ 30°C	[48]
	0.198	@ 40°C	[20]
	0.193	@ 60°C	[20]
	0.184	@ 75°C	[48]
Electrical resistivity:	0.023	MOhm-m @ 18°C	[10],[11]
	0.045	@ 25°C	[11]
Critical temperature:	240.°C	[108],[105],[47],[20],[107],[48]	
	239.49°C		[49]
	239.43°C		[10]
Critical pressure:	9.8		[48]
	8.10		[10],[49]
	7.97		[47]
	7.954		[108],[105]
	7.951		[20]
	7.87	MPa	[107]
Dynamic viscosity:	1.22	mPa-s @ -22.29°C	[105]
	0.970	@ -10°C	[48]
	0.820	@ 0°C	[105]
	0.817	@ 0°C	[48]
	0.623	@ 15°C	[105]
	0.5929	@ 20°C	[49]
	0.593	@ 20°C	[22]
	0.597	@ 20°C	[105]
	0.584	@ 20°C	[48]
	0.5513	@ 25°C	[49]
	0.544	@ 25°C	[10]
	0.547	@ 25°C	[105]

# 380 - Methanol

	0.510	@ 30°C	[105], [48]	
	0.456	@ 40°C	[105]	
	0.403	@ 50°C	[105]	
Kinematic viscosity:	1.54 $\mu\text{m}^2/\text{s}$	@ -22.9°C		
	1.22	@ -10°C		
	1.04	@ 0°C		
	1.03	@ 0°C		
	0.787	@ 15°C		
	0.7491	@ 20°C		
	0.750	@ 20°C		
	0.754	@ 20°C		
	0.738	@ 20°C		
	0.6965	@ 25°C		
	0.691	@ 25°C		
	0.692	@ 25°C		
	0.644	@ 30°C		
	0.576	@ 40°C		
	0.509	@ 50°C		
Surface tension:	24.49 mN/m	@ 0°C air	[105]	
	22.55	@ 20°C	[49]	
	22.6	@ 20°C	[22]	
	22.61	@ 20°C air	[105]	
	22.30	@ 25°C	[49]	
	21.69	@ 30°C	[49]	
	20.14	@ 50°C vapor	[105], [20]	
Contact angle: [18]				
		sessile	advancing	receding
quartz	0	0	0	
calcite	0	0	0	
biotite	0	0	0	
Ca-mont.	0	0	0	
Thermal expansion coefficient:	0.0019 $\text{K}^{-1}$		[48]	
	0.001196		[49]	
Compressibility:	1.078 $\text{nPa}^{-1}$	@ 0°C	[105]	
	1.145	@ 10°C	[105]	
	1.218	@ 20°C	[105]	
	1.248	@ 25°C	[49]	
	1.298	@ 30°C	[105]	
	1.382	@ 40°C	[105]	
	1.476	@ 50°C	[105]	
Vapor diffusivity:	13.2 $\mu\text{m}^2/\text{s}$	@ 0°C	[47]	
Electric dipole moment:	5.64x10 <sup>-30</sup>	C-m	[108]	
	5.67x10 <sup>-30</sup>		[105], [10]	
	9.57x10 <sup>-30</sup>		[49]	
Ionization potential:	10.84 eV (PI, PE)		[105]	
Magnetic volume susceptibility:	-6.66x10 <sup>-6</sup>	SI units @ 20°C	[105]	
Speed of sound:	1189.2 m/s	@ 0°C	[20]	
	1154.9	@ 10°C	[20]	
	1121.2	@ 20°C	[20]	
	1103.	@ 25°C	[105]	
	1088.2	@ 30°C	[20]	
	1055.9	@ 40°C	[20]	
	1024.0	@ 50°C	[20]	

Heat of melting:	3.177 kJ/mol	[105]
	3.179	[107]
	3.215	[49]
	3.22	[10], [48]
Heat of vaporization:	34.5 kJ/mol	[10]
	35.283	[48]
	35.284	[49]
	35.26	[107]
	37.59	[105]
	39.26	[105]
Heat of sublimation:	37.4 kJ/mol	[10]
Heat capacity @ 25°C:	0.08122 kJ/(mol-K) (liq)	[10]
	0.08147 (liq)	[49]
	0.08164 (liq)	[105], [108]
	0.04392 (gas)	[10]
	0.043961 (gas)	[105]
Heat of combustion:	-726.51 kJ/mol @ 25°C (liq)	[49]
	-726.62 (liq)	[20]
	-764.50 (gas)	[49]
	-764.59 (gas)	[20]
	202.4 @ 20°C (sol)	[105]
	-238.66 kJ/mol @ 25°C (liq)	[49]
Heat of formation:	-238.8 (liq)	[105]
	-239.2 (liq)	[10], [20]
	-162.11 (gas)	[105]
	-200.66 (gas)	[49]
	-201.2 (gas)	[10], [20]
	-166.9 kJ/mol @ 25°C (liq)	[10]
Gibbs (free) energy:	-166.47 (liq)	[105]
	-162.5 (gas)	[10]
	11.43 (gas)	[105]
Analytical chemistry: $pP_{oct} =$	-0.82	[104], [21]
	-0.77	[21], [24]
	-0.68	[21]
	-0.66	[104]
	-0.64	[21]
	$pK_s =$ 16.7	[10]
	16.91	[49]
	$pK_a =$ 15.5 @ 25°C	[49]
	$pK_{BH} =$ -2.05 @ 25°C (in aq. $H_2SO_4$ )	[49]
	Henry's law constant = 0.0137 kPa-m <sup>3</sup> /mol @ 25°C	[24]
Hydrolysis half-life = unknown		

**Electrochemical data:** Bagotsky and Vasilyev (1966), Meites and Zuman (1977), Meites et al. (1977b).

**Clay-organic interaction data:** Methanol is reported to both increase and decrease the hydraulic conductivity of clay soil (Anderson et al., 1981, 1985; Foreman and Daniel, 1984; Griffin et al., 1984; Lord et al., 1983). Basal spacing of Ca-montmorillonite complexes with methanol. Interlayer complexes of halloysite with methanol. Complexes formed with rehydrated halloysite obtained by washing the potassium acetate complex with water (Theng, 1974). See also Brindley et al., 1969.

## 382 - Methanol

**Solubility:** Miscible with water, ethanol, ether, acetone, ketones, benzene, and most other organic solvents. [51],[105],[32],[108]

**Form:** Clear, colorless, very mobile, highly polar liquid. Slight alcohol odor when pure. Repulsive, pungent odor from crude material. It is hygroscopic. [51],[108],[22]

**Use:** Industrial solvent; antifreeze for automotive radiators and air brakes; raw material for making formaldehyde and methyl esters; ingredient of gasoline and diesel oil antifreezes; octane booster in gasoline; fuel for portable stoves and torches; extractant for animal and vegetable oils; to denature ethanol; softening agent for pyroxylin plastics; solvent and solvent adjuvant for polymers; solvent in the manufacture of cholesterol, streptomycin, vitamins, hormones, and other pharmaceuticals. [108]

**Fire and explosion hazard:** High.

Flash point: (CC) 11°C [32]  
(CC) 12°C [108],[51],[107],[49]  
(OC) 16°C [107]  
(OC) 15°C [49]  
(OC) 12.2°C [22]

uel: 36% [32]  
36.5% [108],[51],[107],[22]  
lel: 6.0% [108],[51],[107],[22]  
6.7% [32]

Autoign. temp.: 385°C [32]  
464°C [107],[22]  
470°C [108],[51]

Highly flammable liquid with broad range of explosive limits in air. Dangerous fire hazard when exposed to heat, flame, or oxidizers. Moderate explosion hazard when exposed to flame. Can flash back along vapor trail. Toxic gases and vapors (such as carbon monoxide, carbon monoxide, and formaldehyde) may be released in a fire involving methyl alcohol. Can react vigorously with oxidizing materials. Burns with nonluminous bluish flame. Fight fire with alcohol or polymer foam, dry chemical, CO<sub>2</sub>. Water may be ineffective. [51],[32],[108],[107],[55]

**Incompatibility:** Acids; acid chlorides; acid anhydrides; oxidizing agents; reducing agents; and alkali metals; beryllium dihydride; chloroform; cyanuric chloride; metals (especially magnesium); potassium-tert-butoxide; bromine; sodium hypochlorite. Violent reaction with CrO<sub>3</sub>, (I+ethanol+HgO), Pb(ClO<sub>4</sub>)<sub>2</sub>, HClO<sub>4</sub>, P<sub>2</sub>O<sub>3</sub>, (KOH+CHCl<sub>3</sub>), (NaOH+CHCl<sub>3</sub>), nitric acid, hydrogen peroxide, alkylaluminum solutions, diethylzinc, 2,4,6-trichloro-s-triazine. [51],[55]

**Handling:** Keep away from heat, sparks and flame. Avoid breathing vapor or mist. Use in well-ventilated area with supplied-air respirator. Do not use organic canister mask. Avoid eye and skin contact (neoprene, rubber, nitrile, butyl synthetic latex, polyethylene, vinyl plastic, PVC coated nylon gloves and lab coat; safety goggles or face shield). Safety showers and eye wash stations should be supplied. Keep container tightly closed. Bond and ground container when transferring liquid. Store in cool, dry, well-ventilated, flammable liquid storage area. Store in secure poison area. [56],[57],[53]

**Health effects:** Methanol is a poison that possesses distinct narcotic properties to the human system. Routes of entry are inhalation of vapor, percutaneous absorption of liquid, ingestion, and eye and skin contact. Points of attack include eyes, skin, central nervous system, liver, heart, gastrointestinal system. The main toxic effect is exerted upon the nervous system. The first symptoms of overexposure may be blurred vision, photophobia and conjunctivitis, followed by the development of eye lesions. The visual symptoms may clear temporarily, only to return later and progress to blindness. There may also be headache, gastrointestinal disturbances, dizziness and a feeling of intoxication. Irritation of the mucous membranes and peripheral neuritis have been reported. Severe exposures may cause dizziness, unconsciousness, sighing respiration, cardiac depression, convulsions, permanent damage to major organs, and eventually death. The skin may become dry and cracked due to its solvent action. Methanol is slow to be eliminated from the body. Though single exposures to fumes may cause no harmful effects, daily exposure may result in sufficient accumulation in the body to cause illness. It cannot be made non-poisonous. Methanol is a common air contaminant. It is used as a food additive permitted in foods for human consumption. [51],[32],[55],[56]

**Toxicity:** Moderate.

TWA: 200 ppm (260 mg/m<sup>3</sup>) (skin) [1]  
STEL: 250 ppm (310 mg/m<sup>3</sup>) (skin) [1]  
CL: 800 ppm (1050 mg/m<sup>3</sup>) per 15 min [51],[32],[56]  
IDLH: 25000 ppm (31 g/m<sup>3</sup>) [107],[56]  
Peak: 1000 ppm (1300 mg/m<sup>3</sup>) for 30 min duration  
Odor threshold: 100 ppm (130 mg/m<sup>3</sup>) [107]  
2000-5900 ppm (2600-7700 mg/m<sup>3</sup>) [32]  
2000-8000 ppm (2600-10,500 mg/m<sup>3</sup>) [104]  
2000 ppm (2600 mg/m<sup>3</sup>) [56]

Carcinogenicity: unknown

Mutagenicity: unknown

## 384 - Methanol

### Exposure:

#### External:

Non-lethal: 2000 ppm (2.6 g/m<sup>3</sup>) -- virtually nonirritating to the eyes or upper respiratory tract [56]

7500-69000 ppm -- irritation of mucous membranes [32]

Lethal: unknown

#### Oral:

Non-lethal: unknown

Lethal dose: <30 mL [51]

100-250 mL [108]

6.422 mg/kg body wt -- death of an adult male [55]

428 mg/kg body wt -- death of an adult human [55]

143 mg/kg body wt -- death of an adult human [55]

868 mg/kg body wt -- death of an adult male [55]

#### Inhalation:

Short-term Inhalation Limits: 198 ppm (260 mg/m<sup>3</sup>) for 60 min [107]

Non-lethal: 65622 ppm (86 g/m<sup>3</sup>) -- irritant effects (systemic) [51]

1200-8000 ppm (1570-10,500 mg/m<sup>3</sup>) for 4 yrs --

diminution of vision and enlargement of the liver [32]

2000 ppm (2600 mg/m<sup>3</sup>) -- severe toxic effects [104]

500 ppm (660 mg/m<sup>3</sup>) -- symptoms of illness [104]

200 ppm (260 mg/m<sup>3</sup>) -- unsatisfactory [104]

Lethal: 4000-13000 ppm for 12 hrs -- death of an adult female [32]

50000 ppm (66 g/m<sup>3</sup>) for 1 to 2 hours [107]



4-Methyl-2-pentanone

C<sub>6</sub>H<sub>12</sub>O

CAS RN: 108-10-1

Syn: 4-Methyl-2-pentanone \* 2-Pentanone, 4-methyl- \* Hexanone \* Hexone \* Isobutyl methyl ketone \* Isopropylacetone \* Methyl isobutyl ketone \* 2-Methyl-4-pentanone \* 2-Methylpropyl methyl ketone \* MIBK \* MIK \* RCRA Waste Number U161 \* Shell MIBK \* UN 1245 (DOT) \*

Molecular formula: (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>COCH<sub>3</sub>

Aliphatic Ketone

## Physical properties:

Relative molecular mass:	100.161	
Specific gravity:	0.803	[51]
	0.802	[107]
	0.8017	[104]
	0.801	[108]
	0.8010	[49]
	0.8006	[10]
	0.7978	[105]
Boiling point:	119.°C	[104]
	118.°C	[51]
	117.°-118.°C	[56], [108]
	117.4°C	[49]
	116.85°C	[105]
	116.2°C	[107]
	116.°C	[104]
	115.8°C	[22]
	115.7°C	[10]
Melting point:	-80.°C	[104]
	-80.4°C	[22]
	-80.2°C (fp)	[51]
	-83.5°C	[10]
	-84.°C (fp)	[49], [107]
	-84.7°C	[105]
	-85.°C	[104]
Refractive index:	1.3962	[105]
	1.396	[108]
	1.3959	[22]
	1.3958	[10]
	1.39576	[49]
Vapor pressure:	0.1333 kPa @ -1.4°C (1mm)	[105]
	0.800 @ 20°C (6mm)	[104]
	2.09 @ 20°C (15.7mm)	[22]
	2.13 @ 20°C (16mm)	[51]
	2.51 @ 25°C (18.8mm)	[49]
	1.333 @ 30°C (10mm)	[104], [105]
Vapor density:	3.45	[104], [51]
Evaporation rate:	1.62	[49]
Relative dielectric permittivity:	17.37 @ -40°C	[11]
	15.91 @ -10°C	[11]
	14.50 @ 0°C	[11]
	13.11 @ 20°C	[49], [10], [11]
	11.78 @ 40°C	[11]
	9.75 @ 80°C	[11]
	8.90 @ 100°C	[11]

### 386 - 4-Methyl-2-pentanone

Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	>0.19 MOhm-m @ 35°C	[49]
Critical temperature:	298.3°C	[49],[10],[107]
Critical pressure:	3.27 MPa	[49],[10],[107]
Dynamic viscosity:	0.5848 mPa-s @ 20°C	[49]
	0.5463 @ 25°C	[49]
	0.542 @ 25°C	[10]
	0.49751 @ 30°C	[49]
Kinematic viscosity:	0.729 $\mu\text{m}^2/\text{s}$ @ 20°C	
	0.6812 @ 25°C	
	0.676 @ 25°C	
	0.6203 @ 30°C	
Surface tension:	23.6 mN/m @ 20°C	[107]
	23.64 @ 20°C	[49]
	23.29 @ 23.7°C	[49]
	19.62 @ 62.1°C	[49]
Contact angle:	unknown	
Thermal expansion coefficient:	0.000116 K <sup>-1</sup> @	[49]
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	9.30 eV (PI)	[105]
Magnetic volume susceptibility:	-6.96x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	48.8583 kJ/mol	[105]
	35.0	[49]
	34.55	[107]
	41.0 @ 25°C	[49]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.2158 kJ/(mol-K) (liq)	[49],[105]
Heat of combustion:	-3077.8 kJ/mol @ 25°C (liq)	[49]
Heat of formation:	-291.21 @ 25°C (gas)	[49]
Gibbs (free) energy:	unknown	
Analytical chemistry: pP <sub>oct</sub> =	1.09	[41]
	1.19 (est)	[24]
	pK <sub>s</sub> = 25.	[10]
	pK <sub>a</sub> = 4.70	[10]
	pK <sub>BH</sub> = unknown	
Henry's law constant =	0.0095 kPa-m <sup>3</sup> /mol (calc)	[24]
	0.00151 @ 25°C (calc)	[41]
Hydrolysis half-life =	unknown	

Electrochemical Data: Unknown

Clay-organic interaction data: Unknown

**Solubility:** Slightly soluble in water. Soluble in chloroform. Miscible with ethanol, ether, acetone, benzene. [108]

1.9 wt% in water @ 20°C [104]  
1.7 wt% in water @ 25°C [10],[49]

**Form:** Clear, colorless liquid. Pleasant to unpleasant, mild to sharp, sweet ketonic and camphor odor. [108],[107]

**Use:** Manufacture of methyl amyl alcohol; solvent in paints, varnishes, nitrocellulose lacquers; an alcohol denaturant; solvent in uranium extraction from fission products; organic synthesis. [104],[22]

**Fire and explosion hazard:** High.

Flash point: (CC) 23°C [107],[108],[22]

(CC) 16°C [49]

(OC) 24°C [107]

(OC) 23°C [49]

UEL: 7.5% [51],[107],[22]

7.6% [49]

LEL: 1.35% [49]

1.4% [51],[107],[22]

Autoign. temp.: 465°C [49]

460°C [22]

459°C [51]

457°C [107]

Highly flammable liquid. Dangerous fire hazard when exposed to heat, flame, or oxidizers. Moderate explosion hazard when vapor exposed to heat or flame. Flashback along vapor trail can occur. Can react vigorously with reducing materials. Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder. Water may be ineffective. [51],[107],[55]

**Incompatibility:** Violent reaction with potassium *tert*-butoxide. Air; oxidizing agents; reducing agents; strong bases. [55],[51]

**Handling:** Keep away from heat and open flame. Do not breathe vapor or mist (appropriate respirator or self-contained breathing apparatus). Prevent repeated or prolonged eye or skin contact (rubber gloves; laboratory coat; face shield; safety goggles). Employees should wash promptly if skin is wet or contaminated. Remove clothing immediately if wet or contaminated to avoid flammability hazard. Safety shower and eye bath stations should be provided. Use with good ventilation (fume hood). Keep containers tightly closed. Handle containers with nonsparking tools. Store in a cool, dry, well-ventilated flammable liquid storage area. [56],[57],[55]

**Health effects:** Hexone is an irritant with mild narcotic properties. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include respiratory system, eyes, skin, and central nervous system. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. May cause dermatitis, drowsiness, headaches. In high concentrations may cause anesthesia and depression or coma. [56],[55]

### 388 - 4-Methyl-2-pentanone

**Toxicity:** Moderate.

TWA: 50 ppm (205 mg/m<sup>3</sup>) [1]

STEL: 75 ppm (300 mg/m<sup>3</sup>) [1]

CL: unknown

IDLH: 3000 ppm (12,290 mg/m<sup>3</sup>) [56]

Peak: unknown

Odor threshold: 0.47 ppm (1.9 mg/m<sup>3</sup>) [107]

0.07-4.9 ppm (0.3-20 mg/m<sup>3</sup>) -- detection [104]

0.15-15 ppm (0.6-60 mg/m<sup>3</sup>) -- recognition [104]

Carcinogenicity: unknown

Mutagenicity: not genotoxic to mammals [44]

**Exposure:****External:**

Non-lethal: 200 ppm (820 mg/m<sup>3</sup>) for 15 min -- eye irritation [104],[55]

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: unknown

**Inhalation:**

Short-term Inhalation Limits: 100 ppm (410 mg/m<sup>3</sup>) for 60 min [107]

Non-lethal: >100 ppm (410 mg/m<sup>3</sup>) -- headache and nausea [104]

400 ppm (1640 mg/m<sup>3</sup>) -- nasal irritation [104]

Lethal: unknown

Naphthalene

 $C_{10}H_8$ 

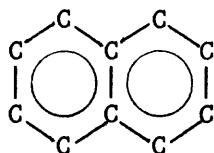
CAS RN: 91-20-3

Syn: Naphthalene \* Albocarbon \* Camphor tar \* Dezodorator \* Mighty 150 \* Mighty RD1 \* Moth balls \* Moth flakes \* Naphthalin \* Naphthaline \* Naphthene \* Naphthalene, molten \* NCI-C52904 \* RCRA Waste Number U165 \* Tar camphor \* UN 1334 (DOT) \* UN 2304 (DOT) \* White tar \*

Molecular formula:  $C_{10}H_8$ 

Polycyclic Aromatic Hydrocarbon

Structural formula:



## Physical properties:

Relative molecular mass:	128.174	
Specific gravity:	1.162	[10], [51], [108]
	1.152	[104]
	1.14	[32]
	1.145	[107], [47], [22], [48]
	1.0253	[105], [106], [14]
Boiling point:	218.°C (sublimes)	[105], [56], [107], [32]
	217.96°C	[22]
	217.955°C	[14]
	217.942°C (sublimes)	[49]
	217.9°C (sublimes)	[104], [51], [108], [48]
	217.7°C	[10]
Melting point:	80.55°C	[105]
	80.5°C	[106]
	80.29°C	[49]
	80.21°C	[14]
	80.2°C	[104], [10], [107], [108], [22]
	80.1°C	[51], [48]
	74.°-80°C	[32], [56]
Refractive index:	1.4003 @ 24°C	[105]
	1.5898 @ 25°C	[106]
	1.5898 @ 85°C	[105], [49], [14]
Vapor pressure:	0.0067 kPa @ 20°C (sol)	(0.05mm) [32]
	0.0109 @ 25°C (sol)	(0.082mm) [49]
	0.1333 @ 52.6°C (sol)	(1mm) [105]
	0.667 @ 74.2°C	(5mm) [47]
	0.997 @ 80.29°C (liq)	(7.48mm) [49]
Vapor density:	4.4	[32]
	4.42	[104], [51]
Evaporation rate:	<<1.	[32]
Relative dielectric permittivity:	2.52 @ 17°-22°C (400 MHz)	[105]
	2.62-2.67 @ 21°C	[2]
	2.54 @ 25°C	[14]
	2.85 @ 25°C	[20]
	2.54 @ 85°C	[49], [10], [105], [20], [11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.377 W/(m-K) @ 0°C	[10]

### 390 - Naphthalene

Electrical resistivity:	23.0 MOhm-m @ 81.8°C	[49]
	23.2 @ 82°C	[11]
	25. @ 82°C	[10]
Critical temperature:	475.28°C	[49]
	475.2°C	[107], [10]
	474.8 C	[105]
Critical pressure:	4.051 MPa	[49], [107], [10]
	4.114	[105]
Dynamic viscosity:	0.967 mPa-s @ 80°C	[105]
	0.776 @ 100°C	[105]
	0.780 @ 100°C	[10]
Kinematic viscosity:	0.832 $\mu\text{m}^2/\text{s}$ @ 80°C	
	0.668 @ 100°C	
	0.672 @ 100°C	
Surface tension:	35.23 mN/m @ 30°C	[14]
	31.52 @ 40°C	[14]
	31.8 @ 100°C	[107], [49]
	27.98 @ 127.2°C	[49]
	28.8 @ 127°C air, vapor	[105]
	18.69 @ 218°C	[49]
Contact angle:	NA	
Thermal expansion coefficient:	0.000283 K <sup>-1</sup> @ 20°C	[48]
Compressibility:	unknown	
Vapor diffusivity:	5.13 $\mu\text{m}^2/\text{s}$ @ 0°C	[47]
Solution diffusivity:	unknown	
Electric dipole moment:	0.	[49], [10]
Ionization potential:	8.12 eV (PI)	[105]
Magnetic volume susceptibility:	-10.3x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	19.31 kJ/mol	[48]
	19.123	[105]
	18.991	[10]
	18.815	[107]
	18.07	[14]
	17.87	[49]
Heat of vaporization:	51.5462 kJ/mol	[105]
	42.21	[14]
	43.32	[107]
	43.292	[10]
	43.18	[49]
	40.25	[48]
Heat of sublimation:	75.513 kJ/mol	[49]
	73.69	[10]
Heat capacity @ 25°C:	0.1658 kJ/(mol-K) (sol)	[108]
	0.1657 (sol)	[49]
	0.1343 (gas)	[108]
	0.1326 (gas)	[10]
Heat of combustion:	5160.4 kJ/mol @ 25°C (sol)	[20]
	5157.3 (sol)	[105]
	5156.95 (sol)	[49]
	5152.7 (sol)	[14]
	5233.12 (gas)	[20]
	5227.5 (gas)	[49]

Heat of formation:	75.362 kJ/mol @ 25°C (sol)	[10]
	78.53 (sol)	[49]
	78.59 (sol)	[20]
	149.0 (gas)	[49]
	149.05 (gas)	[10]
Gibbs (free) energy:	151.3 (gas)	[20]
	201.18 kJ/mol @ 25°C (sol)	[10]
	223.74 (gas)	[10]
Analytical chemistry: $pP_{oct}$ =	4.70	[27]
	3.59	[21]
	3.45	[104], [21]
	3.37	[8], [21]
	3.30	[23], [21], [31]
	3.01	[104], [21]
	$pK_s$ = unknown	
	$pK_a$ = >15.	[59]
	NA	[31]
	$pK_{BH}$ = 4.0 @ 0°C in HF	[49]
Henry's law constant =	0.0365 - 0.0560 kPa-m <sup>3</sup> /mol	[41]
	0.0198 dimensionless	[59]
Hydrolysis half-life =	NA	[8]

**Electrochemical data:** Given and Peover (1960), Klemm et al. (1960), Loveland and Dimeler (1961), Klemm and Kohlik (1963), Klemm et al. (1962), Pysh and Yang (1963), Sternberg et al. (1963), Neikam and Desmond (1964), Neikam et al. (1964), Shriver et al. (1964), Lezhneva and Kruglov (1965), Osa and Kuwana (1969), Wiberg and Lewis (1970), Rieke et al. (1971)

**Clay-organic interaction data:** Intercalation with boiling air-dry samples of montmorillonite (saturated with Ca<sup>2+</sup> or NH<sup>4+</sup> ions) (Theng, 1974). Also see Karickhoff et al. (1970), MacEwan (1948).

**Solubility:** Practically insoluble in water. Soluble in ethanol and methanol. Very soluble in ether, acetone, benzene, toluene, chloroform, carbon tetrachloride, n-heptane, carbon disulfide, hydronaphthalenes, fixed and volatile oils. [51], [105], [32], [10], [104], [49], [47], [14]

0.003 wt% in water @ 20°C	[32]
0.003 vol% in water @ 22°C	[104]
0.003 vol% in water @ 25°C	[47]
0.003169 wt% in water @ 25°C	[49], [23]
69.16 wt% in acetone @ 25°C	[14]
7. wt% in alcohol @ 20°C	[10]
9.5 vol% in alcohol @ 20°C	[47]
12.1 wt% in ethanol @ 25°C	[14]
33. wt% in benzene @ 20°C	[10]
65.71 wt% in benzene @ 25°C	[14]
26.82 wt% in CCl <sub>4</sub> @ 25°C	[14]
50. wt% in CCl <sub>4</sub>	[10]
57.12 wt% in ether @ 25°C	[14]
19.82 wt% in n-heptane @ 25°C	[14]
50. wt% in chloroform	[10]

### 392 - Naphthalene

**Form:** White, crystalline flakes, powder, volatile, balls or cakes.  
Aromatic coal tar odor. Sublimes at room temperature. [51],[108]

**Use:** Manufacture of phthalic and anthranilic acids which are used in making indigo, indanthrene, and triphenylmethane dyes; manufacture of hydroxyl (naphthols), amino (naphthylamines), sulfonic acid and similar compounds used in dye industries; manufacture of synthetic resins, celluloid, lampblack, smokeless powder; manufacture of hydronaphthalenes (Tetralin, Decalin) which are used as solvents, in lubricants, and in motor fuels; preservatives; fungicide. The use as a moth repellent and insecticide is decreasing due to the introduction of chlorinated compounds such as *p*-dichlorobenzene. [108],[56],[104]

**Fire and explosion hazard:** Moderate.

Flash point: (CC) 78.9°C [107]

(CC) 79°C [32]

(CC) 80°C [49]

(CC) 88°C [108]

(OC) 87.8°C [107]

(OC) 79°C [108]

(OC) 78.9°C [51]

uel: 5.9% [32],[51],[107]

lel: 0.9% [32],[51],[107]

Autoign. temp.: 526°C [32],[107],[22]

567°C [51],[108]

Combustible solid. Moderate explosion hazard in the form of dust when exposed to heat or flame. Reacts with oxidizing materials. Reacts violently with CrO<sub>3</sub>. Fire may release dense acrid smoke and CO. Molten naphthalene spatters and foams in contact with water but no chemical reaction is involved. Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder, water fog. Foam and water spray are effective but may cause frothing. [51],[32],[107],[55]

**Incompatibility:** Strong oxidizers; dinitrogen pentaoxide; CrO<sub>3</sub>. [51]

**Handling:** Keep away from heat, sparks and flame. Prevent inhalation of dust, mist or vapor (appropriate respirator or self-contained breathing apparatus recommended). Avoid eye and skin contact (polyethylene, neoprene, PVA synthetic latex, nitrile or PVC coated nylon gloves and lab coat and boots; chemical goggles or face shield). Use in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep containers tightly closed. Store in cool, dry, well-ventilated area. Store under nitrogen. Store in secure poison area or cabinet. [56],[57],[55]



**Health effects:** Naphthalene is a poison. Routes of entry are ingestion, inhalation of vapor or dust, skin absorption, and eye and skin contact. Points of attack include eyes, blood, liver, kidneys, skin, red blood cells, and central nervous system. It is irritating to mucous membranes and upper respiratory tract. On the skin, it may cause hyper-sensitivity dermatitis; chronic dermatitis is rare. The vapors may produce eye irritation, headache, and a warm feeling on the skin with profuse sweating. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. Systemic reactions include nausea, headache, diaphoresis, hematuria, anemia, fever, liver damage, vomiting, convulsions, and coma. Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer. [51],[56],[55],[83],[89]

**Toxicity:** Moderate.

TWA: 10 ppm (50 mg/m<sup>3</sup>) [1]

STEL: 15 ppm (75 mg/m<sup>3</sup>) [1]

IDLH: 500 ppm (2600 mg/m<sup>3</sup>) [107],[56]

Odor threshold: at least as low as 0.3 ppm (1.6 mg/m<sup>3</sup>) [32]

Carcinogenicity: negative [104]

Mutagenicity: experimental equivalent tumorigenic agent [51]  
negative in *Salmonella* test [104]

**Exposure:**

External:

Non-lethal: 15 ppm (79 mg/m<sup>3</sup>) -- eye irritation [32]

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: 29 mg/kg [55]

74 mg/kg [55]

100 mg/kg -- death of a child [55]

Inhalation:

Short-term Inhalation Limits: 15 ppm (79 mg/m<sup>3</sup>) for 5 min [107]

Non-lethal: unknown

Lethal: unknown

## 394 - Nickel

Nickel

Ni

CAS RN: 7440-02-0

Syn: Nickel \* Ni \* Carbonyl nickel powder \* C.I. 77775 \* NI 270 \* Nickel  
 270 \* Nickel (dust) \* Nickel particles \* Nickel sponge \* NI 0901-S \* NI  
 4303T \* NP 2 \* Raney alloy \* Raney nickel \*

Molecular formula: Ni

Element

## Physical properties:

Relative molecular mass:	58.69	[105]
Specific gravity:	8.9	[32], [47], [48]
	8.90 @ 25°C	[105]
	8.90 @ 25°C	[32], [51], [10], [108]
	8.908	[22]
Boiling point:	2730.°C	[51], [32]
	2732.°C	[105]
	2837.°C	[108]
	2900.°C	[22], [47]
	2920.°C	[10]
	3000.°C	[48]
Melting point:	1452.°C	[47]
	1453.°C	[47], [32], [10]
	1455.°C	[10], [22], [51], [105], [48]
	1555.°C	[108]
Refractive index:	NA	
Vapor pressure:	essentially 0. kPa @ 20°C	[32]
	0.133 @ 1810°C (1mm)	[47], [51], [105]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	NA	
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	93.040 W/(m-K) @ 0°C	[48]
	94.1 @ 0°C	[105]
	89.9 @ 25°C	[105]
Electrical resistivity:	6.03x10 <sup>-14</sup> MOhm-m @ 20°C	[105]
	6.84x10 <sup>-14</sup> @ 20°C	[22]
	6.844x10 <sup>-14</sup> @ 20°C	[108]
	7.8x10 <sup>-14</sup> @ 20°C	[105]
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	1735. mN/m @ 1470°C	[105]
	1725. @ m.p. in vacuum	[105]
Contact angle:	NA	
Thermal expansion coefficient:	0.000013 K <sup>-1</sup> @ 20°C	[48]
Compressibility:	NA	
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	NA	
Ionization potential:	7.633 eV (VUS)	[105]
Magnetic volume susceptibility:		
Speed of sound:	5480. m/s long. wave in bulk	[105]

(unmagnetized nickel)	2990.	shear wave in bulk	[105]
	4800.	long. wave in thin rod	[105]
Heat of melting:	17.20 kJ/mol		[48]
	17.58		[105], [47]
	17.63		[10]
	17.94		[108]
Heat of vaporization:	363.67 kJ/mol		[48]
	365.51		[47]
	375.14		[10]
Heat of sublimation:	NA		
Heat capacity @ 25°C:	0.0261 kJ/(mol-K)	(sol)	[10]
	0.0351	(sol)	[105]
	0.0234	(gas)	[10]
Heat of combustion:	NA		
Heat of formation:	0. kJ/mol @ 25°C	(sol)	[105], [10]
	-54.01	(liq-Ni <sup>2+</sup> )	[10]
	-64.06	(liq-Ni <sup>2+</sup> )	[105]
	425.42	(gas)	[105]
	430.0	(gas)	[10]
Gibbs (free) energy:	0. kJ/mol @ 25°C	(sol)	[105], [10]
	-45.64	(liq-Ni <sup>2+</sup> )	[10]
	-46.47	(liq-Ni <sup>2+</sup> )	[105]
	380.04	(gas)	[105]
	384.8	(gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	NA		
pK <sub>s</sub> =	NA		
pK <sub>a</sub> =	9.86 (Ni <sup>2+</sup> )		[10]
pK <sub>BH</sub> =	NA		
Henry's law constant =	NA		
Hydrolysis half-life =	NA		

Electrochemical data: Arvia and Posadas (1975)

Clay-organic interaction data: inorganic

Solubility: Insoluble in hot and cold water. Slightly soluble in HCl, H<sub>2</sub>SO<sub>4</sub>. Soluble in HNO<sub>3</sub>. [32], [47], [105]

Form: A silvery-white, hard, malleable and ductile, somewhat ferromagnetic, odorless metal. It has atomic number 28 (Group VIII) and valence states of +2 or +3. Crystallizes as metallic cubes. A fair conductor of heat and electricity. Occurs free in meteorites and in ores combined with sulfur, antimony, or arsenic. Readily fabricated by hot-and-cold-working. Excellent resistance to corrosion and takes on a high polish. [22], [32], [105], [51], [56]

Use: Used for making stainless steel and other corrosion resistant alloys, coinage, armor plate, electroplating, anodizing aluminum, casting operations for machine parts, acid-resisting and magnetic alloys, magnetic tapes, surgical and dental instruments, catalyst in the hydrogenation of fats and oils, in synthetic coal oil production, as an intermediate in the synthesis of acrylic esters for plastics, colored glass, burglar-proof vaults, colored ceramics, magnets, nickel-cadmium batteries. [105], [56]

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**Fire and explosion hazard:** Very low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable solid. Nickel powder is flammable. Moderate explosion hazard when in the form of dust. Fight fire with dry chemical powder. [51],[55]

**Incompatibility:** Strong acids; aluminium; aluminium trichloride; ethylene; p-dioxan; hydrogen; methanol; non-metals; oxidizing agents; sulfur compounds; wood; F<sub>2</sub>; NH<sub>4</sub>NO<sub>3</sub>; hydrazine; NH<sub>3</sub>; (H<sub>2</sub>+dioxane); performic acid; potassium; selenium; (Ti+KClO<sub>3</sub>). **WARNING:** nickel may react violently with titanium, ammonium nitrate, potassium perchlorate and hydrazoic acid. [51],[56],[55]

**Handling:** Keep away from heat and open flame when in the form of dust. Do not breathe dust or fume (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (leather gloves and suit; safety goggles or face shield). Use of barrier creams to prevent skin sensitization and dermatitis. Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [55],[56],[57]

**Health effects:** Nickel can be highly toxic and is a suspected carcinogen. Routes of entry are inhalation of dust or fumes, ingestion (mostly through food), skin absorption, and eye and skin contact. Points of attack include respiratory system (particularly nasal cavities) and skin. Material is irritating to eyes, skin, mucous membranes, and upper respiratory tract. Symptoms of overexposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. It may cause dermatitis in sensitive individuals. Ingestion of soluble salts causes nausea, vomiting, diarrhea. Nickel fumes may cause pneumonitis. Nickel has been reported to cause cancer of the lungs and sinuses. [51],[32],[56],[55],[84]

**Toxicity:** Low.

TWA: 0.42 ppm (1 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: odorless [32]

Carcinogenicity: animal positive [51],[56]

animal sufficient evidence (IARC cancer review) [55]

Mutagenicity: experimental neoplastic effects [51]

equivocal tumorigenic agent [51]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: 0.11 ppm (0.26 mg/m<sup>3</sup>) for 6 hours -- pneumonitis [51]

Lethal: unknown

## 398 - Nitrobenzene

Nitrobenzene

 $C_6H_5NO_2$ 

CAS RN: 98-95-3

Syn: Nitrobenzene \* Benzene, nitro- \* Essence of mirbane \* Essence of myrbane \* Mirbane oil \* NCI-C60082 \* Nitrobenzene, liquid \* Nitrobenzol \* Nitrobenzol, liquid \* Oil of bitter almonds \* Oil of mirbane \* Oil of myrbane \* RCRA Waste Number U169 \* UN 1662 (DOT) \*

Molecular formula:  $C_6H_5NO_2$ 

Nitro Aromatic Hydrocarbon

## Physical properties:

Relative molecular mass:	123.111	
Specific gravity:	1.19867	[22]
	1.2	[32]
	1.203	[48]
	1.2032	[14]
	1.2037	[105]
	1.20331	[49]
	1.204	[107]
Boiling point:	211.°C	[104], [32], [48]
	210.°-211°C	[51], [108]
	210.9°C	[107], [47]
	210.8°C	[10], [49], [105]
	210.85°C	[22], [14]
Melting point:	6.°C	[104], [51], [108]
	5.8°C	[10]
	5.76°C	[49]
	5.7°C	[105], [47], [48], [22], [14]
	5.1°C (fp)	[107], [32]
Refractive index:	1.5562	[105]
	1.5529	[108]
	1.55230	[14]
Vapor pressure:	0.020 kPa @ 20°C	(0.15mm) [104], [23]
	0.0379 @ 25°C	(0.284mm) [49], [14]
	0.0467 @ 30°C	(0.35mm) [104]
	0.133 @ 44.4°C	(1mm) [105], [51], [47]
Vapor density:	4.25	[104], [51]
	4.3	[32]
Evaporation rate:	unknown	
Relative dielectric permittivity:	35.74 @ 20°C	[11]
	35.75 @ 20°C (1.8 MHz)	[2]
	36.00 @ 24°C (1.2 MHz)	[2]
	35.22 @ 25°C	[2]
	34.89 @ 25°C	[14]
	34.82 @ 25°C	[105], [10], [2], [11]
	34.78 @ 25°C	[49]
	34.62 @ 25°C (10 MHz)	[2]
	34.12 @ 25°C (13.5 MHz)	[2]
	24.9 @ 90°C	[105], [11]
	22.7 @ 110°C	[105]
	20.8 @ 130°C	[105], [11]
Loss tangent:	unknown	
Relaxation time:	unknown	

Thermal conductivity:	0.154 W/(m-K) @ 0°C	[48]	
	0.160 @ 12°C	[48]	
	0.159 @ 12.5°C	[10]	
	0.151 @ 20°C	[48]	
	0.1662 @ 30°-100°C	[105]	
Electrical resistivity:	2. MOhm-m @ 0°C	[10], [11]	
	<50. @ 20°C	[11]	
	48.8 @ 25°C	[49]	
Critical temperature:	482.8°C	[14]	
	459.°C	[49]	
	447.°C	[107]	
Critical pressure:	4.824 MPa	[107]	
Dynamic viscosity:	3.07 mPa-s @ 0°C	[48]	
	2.91 @ 2.95°C	[105]	
	2.71 @ 5.69°C	[105]	
	2.48 @ 9.92°C	[105]	
	2.51 @ 10°C	[48]	
	2.24 @ 14.94°C	[105]	
	2.03 @ 20.00°C	[105]	
	2.01 @ 20°C	[48]	
	1.634 @ 20°C	[10]	
	1.68 @ 30°C	[48]	
Kinematic viscosity:	2.55 $\mu\text{m}^2/\text{s}$ @ 0°C		
	2.42 @ 2.95°C		
	2.25 @ 5.69°C		
	2.06 @ 9.92°C		
	2.09 @ 10°C		
	1.86 @ 14.94°C		
	1.69 @ 20.00°C		
	1.67 @ 20°C		
	1.358 @ 20°C		
	1.40 @ 30°C		
Surface tension:	43.9 mN/m @ 20°C (air or vapor)	[105], [107]	
	43.33 @ 20°C	[14]	
	42.70 @ 20°C	[49]	
	42.17 @ 30°C	[49]	
	41.96 @ 30°C	[14]	
	40.52 @ 40°C	[14]	
Contact angle: [18]			
	sessile	advancing	receding
quartz	33	30	19
calcite	39	33	14
biotite	32	30	11
Ca-mont.	7	12	0
Thermal expansion coefficient:	.0008333 K <sup>-1</sup> @ 25°C	[49]	
Compressibility:	unknown		
Vapor diffusivity:	7.2 $\mu\text{m}^2/\text{s}$ in water	[59]	
	1.00 in CCl4	[47]	
Solution diffusivity:	0.76 nm <sup>2</sup> /s in water	[59]	
Electric dipole moment:	14.10x10 <sup>-30</sup> C-m	[105], [10]	
	13.34x10 <sup>-30</sup>	[49]	
Ionization potential:	9.92 eV (PI)	[105]	
Magnetic volume susceptibility:	-7.59x10 <sup>-6</sup> SI units @ 20°C	[10], [105]	

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Speed of sound:	unknown	
Heat of melting:	11.64 kJ/mol	[10]
	11.63	[49]
	11.60	[107]
	11.59	[14], [105]
	12.11	[48]
Heat of vaporization:	50.9458 kJ/mol	[105]
	50.013 @ 25°C	[49]
	48.97	[48]
	44.32	[107]
	43.45 @ bp	[14]
	40.80 @ bp	[49], [10]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.186 kJ/ (mol-K) (liq)	[10], [48]
@ 30°C:	0.772	[49]
Heat of combustion:	-3094.9 kJ/mol @ 20°C (liq)	[105]
	-3088.08 @ 25°C (liq)	[49]
	-2985.4 (liq)	[107]
Heat of formation:	15.91 kJ/mol @ 25°C (liq)	[10]
	-9.71 (liq)	[49]
Gibbs (free) energy:	146.33 kJ/mol @ 25°C (liq)	[10]
Analytical chemistry: pP <sub>oct</sub> =	1.88	[104], [21]
	1.87	[31]
	1.85	[104], [23], [8], [21], [27]
	1.83	[4]
	1.79	[21]
	pK <sub>s</sub> = unknown	
	pK <sub>a</sub> = 3.98 @ 0°C	[105]
	pK <sub>BH</sub> = unknown	
Henry's law constant =	0.00300 kPa-m <sup>3</sup> /mol	[41]
	0.000626 dimensionless	[59]
Hydrolysis half-life =	NA	[8]

**Electrochemical data:** Meites and Zuman (1977), Meites et al. (1977a), Meites et al. (1977b), Meites et al. (1982), Lund (1983b)

**Clay-organic interaction data:** Nitrobenzene decreases the hydraulic conductivity of kaolinite (Acar et al., 1984, 1985). See also Barshad (1952), Briggs (1981), Greene-Kelly (1955), Yariv et al. (1966).

**Solubility:** Very slightly soluble in water. Very soluble in ethanol, acetone, oils. Miscible with benzene, ether. [108], [10], [104], [32]  
 0.19 vol% in water @ 19°C [104], [49]  
 0.19 wt% in water @ 20°C [10], [32], [47]  
 0.8 wt% in water @ 80°C [104]

**Form:** Bright yellow crystals or light greenish-yellow to light yellow to brown, oily liquid. Bitter almond (or paste shoe polish) odor. Technical grades are 99.5-100% pure. [107], [32].



**Use:** Manufacture of rubber chemicals, drugs, photographic chemicals, aniline, dyes, cellulose acetate; solvent recovery plants; solvent in TNT production, for cellulose ethers; constituent in shoe and floor polishes, leather dressings, paint solvents; masks unpleasant odors; refining lubricant oils. [56],[108],[22]

**Fire and explosion hazard:** Moderate

Flash point: (CC) 87.8°C [107],[22],[51]

(CC) 88°C [49],[32],[108]

(OC) 77.2°C [107]

uel: 40% [55]

lel: 1.8% @ 93.3°C [51]

1.8% [107],[32]

Autoign. temp.: 495.6°C [107]

482°C [51],[32],[22]

Flammable solid or liquid. Toxic gases and vapors (such as nitrogen oxides, CO and CO<sub>2</sub>) may be released in a fire. Volatile with steam. Fight fire with water, alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder. [51],[32],[108],[55]

**Incompatibility:** Strong oxidizing agents; strong reducing agents; strong bases; aluminum trichloride; aniline; glycerol; sulfuric acid; oxidants; phosphorus pentachloride; K; potassium hydroxide; sulfuric acid. Reacts violently with HNO<sub>3</sub>, (AlCl<sub>3</sub> + C<sub>6</sub>H<sub>5</sub>OH); caustic chemically active metals like tin and zinc. **WARNING:** Nitrobenzene forms explosive mixtures with aluminum chloride, aniline and glycerine mixtures, nitric acid, nitrogen tetroxide, and silver perchlorate. A solution of phosphorus pentachloride in nitrobenzene is stable at 110°C but begins to decompose with accelerating violence above 120°C with evolution of nitrous fumes. [51],[32],[56],[55]

**Handling:** Avoid heat, flame, sparks, or sources of ignition. Do not breathe vapor, mist or dust (appropriate respirator or self-contained breathing apparatus). Prevent any possibility of skin and eye contact (rubber gloves; protective overclothing and shoes). Readily absorbed through skin. Wash promptly if skin is wet or contaminated and daily at the end of each work shift. Work clothing should be changed daily if it is possible that clothing is contaminated. Remove nonimpervious clothing immediately if wet or contaminated. Provide emergency showers and eye bath stations. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [56],[57],[55]

**Health effects:** Nitrobenzene is poisonous. Routes of entry are inhalation, ingestion, percutaneous absorption of liquid or vapor, and eye and skin contact. Points of attack include blood, liver, kidneys, spleen, cardiovascular system, central nervous system, and skin. It can cause skin and eye irritation. Liquid and vapor are rapidly absorbed through the skin. Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer. Repeated or prolonged exposure may cause anemia. Nitrobenzene affects the central nervous system producing fatigue, headache, vertigo, vomiting, general weakness, and in some cases severe

## 402 - Nitrobenzene

depression, unconsciousness, and coma. Chronic overexposure may lead to spleen and liver damage, jaundice, liver impairments, and hemolytic jaundice. Exposure to and/or consumption of alcohol may increase toxic effects. A common air contaminant. [51],[32],[56],[55]

### Toxicity: High.

TWA: 1 ppm (5 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 200 ppm (1000 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 5.94 ppm (30 mg/m<sup>3</sup>) [107]

1.9 ppm (9.5 mg/m<sup>3</sup>) [32]

3.6 ppb (0.0182 mg/m<sup>3</sup>) [104]

Carcinogenicity: unknown

Mutagenicity: unknown

### Exposure:

#### External:

Non-lethal: unknown

Lethal: unknown

#### Oral:

Non-lethal: unknown

Lethal: 200 mg/kg -- blood effects in an adult female [51]

#### Inhalation:

Short-term Inhalation Limits: 10 ppm (50 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: 1 ppm (5 mg/m<sup>3</sup>) -- unsatisfactory conditions [104]

6 ppm (30 mg/m<sup>3</sup>) -- headache and vertigo [32]

40 ppm -- symptoms of illness (intoxication) [104],[32]

200 ppm for 60 min -- severe toxic effects [104]

Lethal: unknown

N-Nitrosodiphenylamine

 $C_{12}H_{10}N_2O$ 

CAS RN: 86-30-6

Syn: n-Nitrosodiphenylamine \* Benzenamine, N-nitroso-N-phenyl- \* Curetard A \* Delac J \* Diphenylamine, N-nitroso- \* Diphenylnitrosamine \* Diphenyl N-nitrosoamine \* N,N-Diphenylnitrosamine \* Naugard TJB \* NCI-C02880 \* NDPA \* NDPHA \* Nitrosodiphenylamine \* N-Nitroso-N-phenylaniline \* Nitrous diphenylamide \* Redax \* Retarder J \* TJB \* Vulcalent A \* Vulcatard \* Vulcatard A \* Vulkalent A \* Vultrol \*

Molecular formula:  $(C_6H_5)_2N-NO$ 

Aromatic Amine

**Physical properties:**

Relative molecular mass:	198.224	
Specific gravity:	1.23	[22]
Boiling point:	unknown	
Melting point:	144.0°C	[51]
	145.°C	[22]
	66.°-67°C	[10]
	66.5°C	[105]
	64.-66°C	[22]
Refractive index:	unknown	
Vapor pressure:	0.13 kPa @ 25°C (0.1mm)	[31]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	unknown	
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	unknown	
Heat of combustion:	-6416.7 kJ/mol @ 20°C (sol)	[105]
Heat of formation:	213.1 kJ/mol @ 25°C	[10]
Gibbs (free) energy:	unknown	

Analytical chemistry:  $pP_{oct}$  = 3.13 [4]. [27], [31], [41]  
 2.57 [8]  
 $pK_s$  = NA

#### 404 - N-Nitrosodiphenylamine

pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	2.36x10 <sup>-6</sup> kPa-m <sup>3</sup> /mol @ 25°C	[41]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

**Solubility:** Slightly soluble in water. Soluble in ether, benzene, ethanol. Very soluble in chloroform, hot ethanol, hot benzene, ether. [10],[105],[55]

0.0035 wt% in water @ 25°C [41]

**Form:** Green or dark blue crystals; yellow to brown or orange powder or flakes. [22],[51],[41]

**Use:** Retarder of vulcanization in rubber; pesticide; chemical intermediate for *N*-phenyl-*p*-phenylenediamine. [22],[41]

**Fire and explosion hazard:** Very low.

Flash point: NA

lel: NA

Autoign. temp.: NA

Nonflammable solid. Emits highly toxic fumes of CO, CO<sub>2</sub>, and nitrogen oxides when heated to decomposition. [51]

**Incompatibility:** Oxidizing agents. [51],[55]

**Handling:** Avoid heat and flame. Do not inhale dust, mist or vapor (appropriate respirator or self-contained breathing apparatus). Avoid all contact with skin, eyes, and clothing (long rubber or neoprene gauntlet gloves; chemical safety goggles; over-clothing). Keep container tightly closed. Store in a cool, dry, secure poison storage area or cabinet. Handle in a closed system. [56],[55]

**Health effects:** NDPA may be an irritant and is a suspected carcinogen. Routes of entry are inhalation, ingestion, and skin absorption. Points of attack include skin and eyes. May cause skin and eye irritation. Nitrosamines are suspected of causing cancers of the lung, nasal sinuses, brain, esophagus, stomach, liver, bladder and kidney. [51],[55]

**Toxicity:** Low

TWA: no values set [1]

STEL: no values set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: probable [22],[51]  
limited animal evidence [55]

Mutagenicity: suspected [51]  
tested positive [109]

**Exposure:** Unknown

Pentachlorophenol

 $C_6HCl_5O$ 

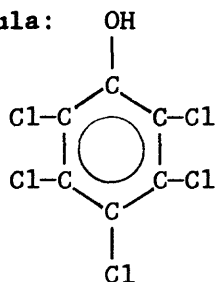
CAS RN: 87-86-5

Syn: Pentachlorophenol \* Phenol, pentachloro- \* Acutox \* Chem-penta \* Chem-tol \* Chlon \* Chlorophen \* Cryptogil OL \* Dowside EC-7 \* Dowcide G Dowcide 7 \* Dowicide 7 \* Dow pentachlorophenol DP-2 antimicrobial \* Durotox \* EP 30 \* Fungifen \* Glazd Penta \* Grundier arbezol \* Lauxtol \* Lauxtol A \* Liroprem \* Monsanto Penta \* Moosuran \* NA 2020 (DOT) \* NCI-C54933 \* NCI-C55378 \* NCI-C56655 \* PCP \* PCP (pesticide) \* Pencilorol \* Penta \* Pentachlorofenol \* Pentachlorophenate \* 2,3,4,5,6-Pentachlorophenol \* Pentachlorophenol, Dowicide EC-7 \* Penta-chlorofendo \* Pentachlorophenol, DP-2 \* Pentacon \* Penta-kil \* Pentasol \* Penwar \* Peratox \* Permacide \* Permagard \* Permasan \* Permattox DP-2 \* Permattox Penta \* Permitte \* PKhF \* Prevenol P \* Priltox \* RCRA Waste Number U242 \* Santobrite \* Santophen \* Santophen 20 \* Sinituho \* Term-i-trol \* Thompson's Wood Fix \* Weedone \* Witophen \* Witophen P \*

Molecular formula:  $C_6Cl_5OH$ 

Polychlorinated Phenol

Structural formula:



Physical properties:

Relative molecular mass:	266.338	
Specific gravity:	1.978	[104], [51]
	1.98	[107]
	2.0	[32]
Boiling point:	311.°C	[32]
	310.°C decomposes	[10], [104], [51], [22]
	309.°-310°C	[108]
Melting point:	191.°C	[104], [105], [51]
	190.°-191°C	[10], [108]
	190.°C	[22]
	187.°-189°C	[56]
	182.°-190°C	[32]
	188.°C (fp)	[104], [107]
Refractive index:	unknown	
Vapor pressure:	1.47x10 <sup>-5</sup> kPa @ 20°C (0.00011mm)	[104]
	2.2x10 <sup>-5</sup> @ 20°C (0.00017mm)	[32]
	5.333 @ 211.2°C (40mm)	[105], [51]
Vapor density:	9.20	[104]
Evaporation rate:	unknown	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	

## 406 - Pentachlorophenol

Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	5.2 $\mu\text{m}^2/\text{s}$ (calc)	[59]
Solution diffusivity:	0.56 $\text{nm}^2/\text{s}$ (calc)	[59]
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	17.15 kJ/mol	[105]
Heat of vaporization:	70.098 kJ/mol	[105]
Heat of sublimation:	67.41 kJ/mol	[10]
Heat capacity @ 25°C:	0.202 kJ/(mol-K) (sol)	[10]
Heat of combustion:	NA	
Heat of formation:	-295.6 kJ/mol @ 25°C (sol)	[10]
Gibbs (free) energy:	-144.2 kJ/mol @ 25°C (sol)	[10]
Analytical chemistry: $pP_{\text{oct}}$ =	5.86	[21]
	5.12	[21]
	5.04	[31]
	5.01	[104], [8], [21]
	$pK_s$ = unknown	
$pK_a$ =	4.74	[8], [31]
$pK_{BH}$ =	unknown	
Henry's law constant =	0.00034 kPa-m <sup>3</sup> /mol	[41]
	0.00021	[41]
	0.000028	[41]
	0.00036 dimensionless	[59]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Choi and Aomine (1974), Kenega and Goring (1980), Nose (1966).

Solubility: Almost insoluble in water. Slightly soluble in cold petroleum ether and hydrocarbons. Soluble in ether, benzene, dilute alkali, pine oil. Very soluble in ethanol. [51], [22], [10], [104], [32]

0.0005 wt% in water @ 0°C	[104]
0.0014 wt% in water @ 20°C	[104]
0.002 wt% in water @ 20°C	[32]
0.019 wt% in water @ 30°C	[41]
0.003 wt% in water @ 50°C	[10]
0.0035 wt% in water @ 50°C	[104]
0.0085 wt% in water @ 70°C	[104]
14.8 wt% in ether @ 25°C	[10]

**Form:** Colorless, white, light-brown, dark-gray to brown beads or flakes and sublimed needle crystals. Weak, characteristic phenolic-like odor. Pungent when hot. Commercial PCP contains significant quantities, up to 40%, of tetrachlorophenol (TCP). Technical PCP has been reported to contain chlorodiphenylethers, chlorodibenzo-*p*-dioxins, chlorodibenzofurans, hydroxychlorodiphenylethers, and octachlorodibenzo-*p*-dioxin. [104],[51],[32]

**Use:** Used primarily as a wood and wood product preservative; manufacture of insecticides, fungicides, bactericides, slimicides, contact herbicides, algicides, mulluscicides; manufacture of sodium pentachlorophenate. [56],[108],[22],[104]

**Fire and explosion hazard:** Very low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable solid. Emits highly toxic fumes (such as hydrogen chloride, chlorinated phenols, and CO) when heated to decomposition. Fight fire with CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [51],[32],[107],[55]

**Incompatibility:** Strong oxidizing agents; strong bases; acid chlorides; acid anhydrides. [32],[56],[55]

**Handling:** Avoid heat and flame. Prevent inhalation of dust, mist, or vapor (appropriate respirator or self-contained breathing apparatus). Prevent any possibility of skin and eye contact (rubber gloves; laboratory coat; safety goggles). It is readily absorbed through skin. Use with adequate ventilation (fume hood). Employees should wash immediately when skin is wet or contaminated. Work clothing should be changed daily if it is possible that clothing is contaminated. Remove nonimpervious clothing immediately if wet or contaminated. Provide emergency showers and eye wash stations. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [56],[55]

**Health effects:** PCP is a poison. Routes of entry are inhalation of dust, skin absorption, ingestion, and eye and skin contact. Points of attack include cardiovascular system, respiratory system, eyes, liver, kidneys, skin, and central nervous system. It is irritating to mucous membranes and upper respiratory tract. Liquid or solid causes smarting of the skin and first-degree burns on short exposure; may cause second degree burns on long exposure. Also causes dermatitis, convulsions and collapse. Dust causes sneezing. Acute poisoning is marked by weakness and respiratory, blood pressure and urinary output changes, and may be fatal. Chronic exposure can cause liver and kidney injury. May cause congenital malformation in the fetus. Intoxication is characterized by weakness, anorexia, weight loss, and profuse sweating; there also may be headache, dizziness, nausea, vomiting, dyspnea, and chest pain. The risk of serious intoxication is increased during hot weather. [51],[32],[107],[55],[85]

#### 408 - Pentachlorophenol

**Toxicity:** Moderate to high.

TWA: 0.046 ppm (0.5 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 14 ppm (150 mg/m<sup>3</sup>) [56],[107]

Peak: unknown

Odor threshold: very weak odor [107]

Carcinogenicity: indefinite [51]

considered not to be carcinogenic [56]

Mutagenicity: equivocal tumorigenic agent by RTECS criteria [55]

possible teratogen [55]

#### **Exposure:**

##### **External:**

Non-lethal: 0.09 ppm (1 mg/m<sup>3</sup>) -- painful irritation to eyes, nose,  
throat, and upper respiratory tract [104]

0.03 ppm (0.3 mg/m<sup>3</sup>) -- nose irritation [32]

Lethal: unknown

##### **Oral:**

Non-lethal: 196 mg/kg -- CNS effects in an adult male [51]

Lethal: 29 mg/kg -- death of an adult human [51]

401 mg/kg [55]

##### **Inhalation:**

Short-term Inhalation Limits: unknown

Non-lethal: 0.22 ppm (2.4 mg/m<sup>3</sup>) -- tolerable concentration for  
acclimated persons [32]

Lethal: unknown



Phenanthrene

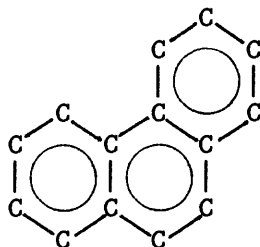
 $C_{14}H_{10}$ 

CAS RN: 85-01-8

Syn: Phenanthrene \* Phenanthren \* Phenantrin \*

Structural formula:

Polynuclear Aromatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	178.233	
Specific gravity:	1.179 @ 25°C	[10], [51], [47], [108]
	1.063	[22]
	1.025	[104]
	0.9800 @ 4°C	[106], [105], [59]
Boiling point:	340.°C	
	[104], [106], [105], [10], [47], [22], [108]	
	339.°C	[51]
Melting point:	101.°C	[105], [106]
	100.35°C	[22]
	100.°C	[10], [104], [51], [108]
	99.°-100°C	[47]
Refractive index:	1.5943	[105], [106]
Vapor pressure:	0.1333 kPa @ 118.3°C (1mm)	[105], [51]
	0.9x10 <sup>-4</sup> @ 20°C (6.8x10 <sup>-4</sup> mm)	[86]
	2.8x10 <sup>-5</sup> @ 20°C (2.1x10 <sup>-4</sup> mm)	[41]
	1.3x10 <sup>-4</sup> @ 25°C (9.6x10 <sup>-4</sup> mm)	[31]
Vapor density:	6.14	[51]
Evaporation rate:	unknown	
Relative dielectric permittivity:	2.8 @ 20°C	[11]
	2.83 @ 21°C	[2]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	8.1 eV (EI)	[105]
Magnetic volume susceptibility:	-9.59x10 <sup>-6</sup> SI units @ 100°C	[105]
Speed of sound:	unknown	
Heat of melting:	16.47 kJ/mol	[105]
Heat of vaporization:	59.386 kJ/mol	[105]

## 410 - Phenanthrene

	55.68	[10]
Heat of sublimation:	88.34 kJ/mol	[10]
Heat capacity @ 25°C:	unknown	
Heat of combustion:	-7057.3 kJ/mol @ 25°C (sol)	[105]
Heat of formation:	114.30 kJ/mol @ 25°C (sol)	[10]
Gibbs (free) energy:	268.46 kJ/mol @ 25°C (sol)	[10]

Analytical chemistry:	pP <sub>oct</sub> -	4.46	[104],[8],[21],[27].[31],[59]
	pK <sub>s</sub> -	NA	
	pK <sub>a</sub> -	>15.	[59]
		NA	[31]
	pK <sub>BH</sub> -	NA	
Henry's law constant -		0.013 kPa-m <sup>3</sup> /mol	[41]
		0.00555	[41]
		0.0039	[41]
		0.00259 @ 25°C	[41]
		0.00615 dimensionless (calc)	[59]
Hydrolysis half-life -		NA	[8]

**Electrochemical data:** Unknown

**Clay-organic interaction data:** Karickhoff et al. (1979)

**Solubility:** Almost insoluble in water. Soluble in acetone, ethanol, CS<sub>2</sub>, benzene, hot ethanol, chloroform, glacial acetic acid. Very soluble in ether. [10],[51],[105],[10],[104]

0.423 ppm in water @ 8.5°C	[104]
0.00016 wt% in water @ 15°C	[104]
0.816 ppm in water @ 21°C	[104]
1.277 ppm in water @ 30°C	[104]
2. wt% in ethanol	[10]
50. wt% in benzene	[10]
30. wt% in ether	[10]

**Form:** Solid, monoclinic, shining crystals or colorless leaflets. [51],[104],[22]

**Use:** Dyestuffs; explosives; drug synthesis; biochemical research. Present in commercial coal tar and gasoline. Can be found in any hydrocarbon combustion process and may be released from oil spills. [107],[22]

**Fire and explosion hazard:** Low.

Flash point: (OC) 171°C [41]

uel: unknown

lel: unknown

Autoign. temp.: unknown

Slightly flammable solid. When heated to decomposition it emits acrid smoke and fumes, including CO and CO<sub>2</sub>. To fight fire use water, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [51],[55]

**Incompatibility:** Strong oxidizing agents. [55]

**Handling:** Avoid heat and flame. Avoid inhalation of dust, fumes, or mist (appropriate respirator or self-contained breathing apparatus). Prevent contact with skin, eyes and clothing (rubber gloves; laboratory coat; safety goggles). Use with good ventilation (fume hood). Safety shower and eye bath should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [57],[55]

**Health effects:** Phenanthrene is an irritant and possible carcinogen. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include respiratory tract, eyes, and skin. It is irritating to skin, eyes, mucous membranes, and upper respiratory tract. A human skin photosensitizer. Exposure to light can result in allergic reactions resulting in dermatologic lesions, which can vary from sunburn-like responses to edematous, vesiculated lesions or bullae. The chemical, physical, and toxicological properties have not been thoroughly investigated. [51],[55],[86]

**Toxicity:** Low.

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: 0.0076-0.0082 ppm (0.055-0.06 mg/m<sup>3</sup>) [104]

Carcinogenicity: negative [104],[86]  
carcinogenic agent [22]

Mutagenicity: experimental neoplastic effects, equivocal tumorigenic agent [51]  
negative in the *Salmonella* test [104]

**Exposure:** Unknown

External:

Non-lethal: NA

Lethal: NA

Oral:

Non-lethal: NA

Lethal: NA

Inhalation:

Short-term Inhalation Limits: NA

Non-lethal: NA

Lethal: NA

## 412 - Phenol

Phenol

 $C_6H_6O$ 

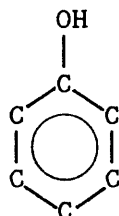
CAS RN: 108-95-2

Syn: Phenol \* Baker's P and S liquid and ointment \* Benzenol \* Carbolic acid \* Hydroxybenzene \* Monohydroxybenzene \* Monophenol \* NA 2821 (DOT) \* NCI-C50124 \* Oxybenzene \* Phenic acid \* Phenol alcohol \* Phenol, molten \* Phenol, liquid or solution \* Phenyl hydrate \* Phenyl hydroxide \* Phenylic acid \* Phenylic alcohol \* RCRA Waste Number U188 \* UN 1671 (solid) (DOT) \* UN 2312 (molten) (DOT) \* UN 2821 (solution) (DOT) \*

Molecular formula:  $C_6H_5OH$ 

Phenol

Structural formula:



## Physical properties:

Relative molecular mass:	94.1128	
Specific gravity:	1.05 (liq)	[32]
	1.0576 (sol)	[105], [106]
	1.05760 @ 41°C	[10], [14]
	1.058 @ 41°C (liq)	[107]
	1.07 (sol)	[32], [22]
	1.070	[104]
	1.071 (liq)	[51], [47], [10], [108]
	1.072 (sol)	[51]
Boiling point:	182.°C	[104], [32], [22], [108]
	181.7°C	[105]
	181.9°C	[51]
	181.839°C	[49]
	181.8°C	[107], [10]
	181.75°C	[14]
	181.4°C	[47]
	43.°C	[105], [106]
Melting point:	42.5-43°C	[22]
	42.°-43°C	[47]
	41.°C	[32], [104], [56]
	40.90°C	[49], [107], [10], [14]
	40.85°C	[108]
	40.6°C	[51]
	1.54274 @ 40.6°C	[49]
	1.5418 @ 41°C	[10]
Refractive index:	1.5408 @ 41°C	[105], [106]
	0.027 kPa @ 20°C (0.2mm)	[104]
Vapor pressure:	0.0480 @ 20°C (0.36mm)	[32]
	0.055 @ 25°C (0.41mm)	[49]
	0.070 @ 25°C (0.52mm)	[23]
	0.1333 @ 40.1°C (1mm)	[51], [47], [20]
	3.24	[32], [51], [104]
Vapor density:		
Evaporation rate:	<0.01	[32]

Relative dielectric permittivity:	4.3 @ 10°C (400 MHz)	[105]
	9.8 @ 21°C	[2]
	11.60 @ 40°C	[49]
	10.28 @ 50°C (1 MHz)	[2]
	9.78 @ 60°C	[105],[10],[11]
	10.00 @ 60°C	[49]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.149 W/(m-K) @ 30°C	[49]
	0.141 @ 75°C	[49]
Electrical resistivity:	<0.59 Mohm-m @ 25°C	[10],[11]
	0.373 @ 50°C	[49]
Critical temperature:	419.0°C	[47]
	419.25°C	[20]
	421.1°C	[49],[10],[107],[105]
Critical pressure:	6.130 MPa	[10],[20],[49],[107],[105]
Dynamic viscosity:	12.7 mPa-s @ 18.3°C	[105]
	12.4 @ 20°C	[48]
	7.50 @ 30°C	[48]
	5.11 @ 40°C	[48]
	4.076 @ 45°C	[49]
	3.67 @ 50°C	[48]
	3.49 @ 50°C	[105]
	2.61 @ 60°C	[105]
	2.03 @ 70°C	[105]
	1.26 @ 90°C	[105]
Kinematic viscosity:	12.01 $\mu\text{m}^2/\text{s}$ @ 18.3°C	
	11.6 @ 20°C	
	7.0 @ 30°C	
	4.77 @ 40°C	
	3.854 @ 45°C	
	3.43 @ 50°C	
	3.30 @ 50°C	
	2.47 @ 60°C	
	1.92 @ 70°C	
	1.19 @ 90°C	
Surface tension:	40.9 mN/m @ 20°C air, vapor	[105],[47]
	39.88 @ 30°C air, vapor	[105]
	37.66 @ 50°C	[15]
	37.77 @ 50°C	[49]
	37.26 @ 55°C	[49]
	36.57 @ 60°C	[15]
	36.69 @ 60°C	[49]
	35.51 @ 70°C	[15]
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	0.561 nPa <sup>-1</sup> @ 46°C	[105]
	0.605 @ 60°C	[105]
	0.678 @ 80°C	[105]
Vapor diffusivity:	8.2 $\mu\text{m}^2/\text{s}$ (calc)	[59]

## 414 - Phenol

Solution diffusivity:	0.85 nm <sup>2</sup> /s in water (calc)	[59]
	0.2 in i-amyl alcohol	[47]
	1.68 in benzene	[47]
	3.7 in carbon disulfide	[47]
	2.0 in chloroform	[47]
	0.89 in ethanol	[47]
Electric dipole moment:	3.9 in ethyl ether	[47]
	4.837x10 <sup>-30</sup> C-m	[105], [10]
	5.30x10 <sup>-30</sup> @ 30°C	[49]
	7.34x10 <sup>-30</sup> @ 40°C	[49]
Ionization potential:	8.51 eV (PI)	[105]
Magnetic volume susceptibility:	-8.48x10 <sup>-6</sup> SI units @ 45°C	[105]
Speed of sound:	unknown	
Heat of melting:	11.514 kJ/mol	[49]
	11.52	[10]
	11.289	[105]
Heat of vaporization:	40.73 kJ/mol	[10]
	45.689	[49]
	49.79	[105]
Heat of sublimation:	68.659 kJ/mol	[49]
	68.71	[10]
Heat capacity @ 25°C:	0.12721 kJ/(mol-K) (sol)	[49]
	0.1348 (sol)	[10]
	0.1275 (liq)	[10]
	0.1032 (gas)	[49]
	0.1036 (gas)	[10]
Heat of combustion:	-3053.48 kJ/mol @ 25°C (sol)	[49]
	-3055.5 (sol)	[105]
Heat of formation:	-165.06 kJ/mol @ 25°C (sol)	[49]
	-165.1 (sol)	[10], [20]
	-158.3 (liq)	[10]
	-96.21 (gas)	[20]
	-96.399 (gas)	[49]
	-96.42 (gas)	[10]
	-50.45 kJ/mol @ 25°C (sol)	[10]
Gibbs (free) energy:	-46.14 (liq)	[10]
	-32.91 (gas)	[10]
Analytical chemistry:	pP <sub>oct</sub> = 1.51	[21]
	1.48	[31]
	1.46	[104], [23], [8], [21], [59]
	pK <sub>s</sub> = unknown	
	pK <sub>a</sub> = 9.686 @ 20°C	[49]
	9.89 @ 20°C	[31]
	10.0 @ 25°C	[108], [8]
	9.99 @ 25°C	[10], [23]
	9.92 @ 25°C	[11]
	9.89 @ 25°C	[105]
	9.658 @ 30°C	[49]
	14.0 in methanol	[10]
	pK <sub>BH</sub> = unknown	

Henry's law constant =	0.0000402 kPa-m <sup>3</sup> /mol @ 25°C	[41]
	0.000027	[41]
	0.0000173	[41]
	0.000054 dimensionless	[59]
Hydrolysis half-life =	NA	[8]

**Electrochemical data:** Suatoni et al. (1961), Turner and Elving (1965), Pungor and Szepesvary (1968), Tsuji and Elving (1969), Meites and Zuman (1977), Meites et al. (1977a), Anderson and Stocker (1983), Ebersson and Utley (1983a), Hammerich (1983), Simonet (1983).

**Clay-organic interaction data:** Phenol is reported to both increase and decrease the hydraulic conductivity of clay soils (Acar et al., 1985). Interlayer expansions in vermiculite due to intercalated phenols. Water molecules reacting as bases and accepting protons from acids through hydrogen bonding by sorption of phenol on Al-montmorillonite. (Yariv and Cross, 1979 and Theng, 1974). Also see Acar et al., 1985; Artiola-Fortung and Fuller, 1982; Erickson, 1948; Fenn and Mortland, 1973; Greene-Kelly, 1955; Isaacson and Sawhney, 1983; Kenega and Goring, 1980; Wang et al., 1978.

**Solubility:** Almost insoluble in petroleum ether. Soluble in water, benzene. Very soluble in ethanol, ether, chloroform, carbon tetrachloride, glycerol, carbon disulfide, petrolatum, volatile and fixed oils, aqueous alkali hydroxides. Miscible with water above 65.3°C. [10],[22],[108],[14],[104],[32],[49],[47]

6.7 wt% in water @ 20°C	[10]
8.2 wt% in water @ 15°C	[104]
8.4 wt% in water @ 20°C	[32]
8.66 wt% in water @ 25°C	[49]
8.20 wt% in water @ 25°C	[14]
8.2 wt% in benzene	[10]

**Form:** Colorless, acicular crystals or white, crystalline mass which turns pink or red if not perfectly pure or under the influence of light. Absorbs water from the air and liquefies. Characteristic sweet, tarry, odor; burning taste. When in very weak solution it has a sweetish taste. Weak organic acid. [51],[107],[22],[108]

**Use:** As a general disinfectant, either in solution or mixed with slaked lime, etc., for toilets, stables, cesspools, floors, drains, etc.; manufacture of colorless or light-colored resins, many medical and industrial organic compounds and dyes; as a reagent in chemical analyses; germicidal paints; 2,4-D; salicylic acid; adipic acid; selective solvent for refining lubricating oils. Present in gasoline engine exhaust (1-2 ppm). [108],[22],[56],[104]

## 416 - Phenol

**Fire and explosion hazard:** Moderate.

Flash point: (CC) 78°C [22]  
(CC) 79°C [32],[49],[108]  
(CC) 79.4°C [107],[51]  
(OC) 85°C [107]

uel: 8.6% [32],[107]

lel: 1.7% [32],[107]

Autoign. temp.: 715°C [32],[51],[107],[22]

Combustible liquid. Moderate fire hazard when exposed to heat, flame or oxidizers. Dangerous when heated as it emits toxic fumes (such as carbon monoxide). Moderate explosion hazard as it yields flammable vapors when heated which will form explosive mixtures with air. Gives off heavy smoke. Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder, water spray. [51],[32],[107]

**Incompatibility:** Contact with strong oxidizers (especially calcium hypochlorite); formaldehyde, NaNO<sub>2</sub>, NaNO<sub>3</sub>, tri-fluoroacetic acid. Reacts violently with (AlCl<sub>3</sub> + nitrobenzene), butadiene, peroxydisulfuric acid, peroxymonosulfuric acid. [32],[108],[56]

**Handling:** Keep away from heat, sparks and flame. Avoid breathing vapor (appropriate chemical respirator or self-contained breathing apparatus). Do not get in eyes, skin or clothing (neoprene, rubber, latex or nitrile gloves; lab coat and apron; safety goggles and face shield). Use in well-ventilated area (fume hood). Keep container tightly closed. Store in cool, dry, well-ventilated, flammable liquid storage area or cabinet. [57],[56],[107],[53]

**Health effects:** Phenol is a poison and potential carcinogen. Routes of entry are inhalation of mist or vapor, percutaneous absorption of mist, vapor or liquid, ingestion, and eye and skin contact. Points of attack include liver, kidneys, pancreas, spleen, respiratory system, gastrointestinal system, nervous system, and skin. It is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. In acute phenol poisoning, the main effect is on the CNS. Absorption from spilling phenolic solutions on the skin may be very rapid, and death results from collapse within 30 minutes to several hours. Where death is delayed, damage to the kidneys, liver, pancreas and spleen and edema of the lungs may result. The symptoms develop rapidly, frequently within 15-20 minutes following spilling phenol on the skin. Headache, dizziness, muscular weakness, dimness of vision, ringing in the ears, irregular and rapid breathing, weak pulse, and dyspnea may all develop, and may be followed by loss of consciousness, collapse and death. When taken internally there is also nausea, with or without vomiting, severe abdominal pain, and corrosion of the lips, mouth, throat, esophagus and stomach. On the skin the affected area is white, wrinkled and softened, and there is usually no immediate complaint of pain; later intense burning is felt, followed by local anesthesia and still later by gangrene. Chronic poisoning, following prolonged exposures to low concentrations of the vapor



or mist, results in digestive disturbances, nervous disorders and skin eruptions. Chronic poisoning may terminate fatally in cases where there has been extensive damage to the liver or kidneys. Dermatitis resulting from contact with phenol or phenol-containing products is fairly common in the industry. A common air contaminant. [51],[32],[56],[87]

**Toxicity:** High.

TWA: 5 ppm (19 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: 16 ppm (60 mg/m<sup>3</sup>) for 15 min [51],[32],[56]

IDLH: 100 ppm (385 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 0.05 ppm (0.2 mg/m<sup>3</sup>) [107]

0.1-5 ppm (0.4-19 mg/m<sup>3</sup>) [32]

0.0478 ppm (0.184 mg/m<sup>3</sup>) [104]

Carcinogenicity: results negative [51]

carcinogenic in laboratory animals [107]

Mutagenicity: experimental carcinogen, neoplastic effects, equivocal tumorigenic agent [51]

**Exposure:**

External:

Non-lethal: unknown

Lethal: Death has resulted from absorption of phenol through a skin area of 64 square inches. [32]

Oral:

Non-lethal: unknown

Lethal: 1-10 g [32]

1-15 g [56]

1 g [104]

10 mg/kg -- death of an infant [55]

14 g/kg [55]

140 mg/kg [55]

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: 48 ppm (185 mg/m<sup>3</sup>) -- nose and throat irritation [32]

Lethal: unknown

## 418 - Potassium Cyanide

Potassium Cyanide

KCN

CAS RN: 151-50-8

Syn: Potassium cyanide \* Cyanide of potassium \* Hydrocyanic acid \*  
 Hydrocyanic acid, potassium salt \* Potassium salt \* RCRA Waste Number P098  
 \* UN 1680 (DOT) \*

Molecular formula: KCN

Cyanide

## Physical properties:

Relative molecular mass:	65.1199	
Specific gravity:	1.52 @ 16°C	[22],[105],[47],[10]
Boiling point:	1625.°C	[51],[10]
Melting point:	635.°C	[32]
	634.5°C	[105],[47]
	622.°C	[10]
Refractive index:	1.410	[47],[105],[10]
Vapor pressure:	0. kPa @ 20°C	[32]
Vapor density:	NA	[32]
Evaporation rate:	NA	[32]
Relative dielectric permittivity:	6.2	[11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	NA	[107]
Critical pressure:	NA	[107]
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	[107]
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	-465.0x10 <sup>-6</sup> SI units	[105]
Speed of sound:	unknown	
Heat of melting:	14.6 kJ/mol	[10],[20],[105]
Heat of vaporization:	157.2 kJ/mol	[10]
Heat of sublimation:	192. kJ/mol	[10]
Heat capacity @ 25°C:	0.0664 kJ/(mol-K) (sol)	[10],[105]
	0.0524 (gas)	[10],[105]
Heat of combustion:	NA	[107]
Heat of formation:	-113.04 kJ/mol @ 25°C (sol)	[10],[105]
	-117.6 (sol)	[57]
	90.85 (gas)	[10],[105]
Gibbs (free) energy:	-101.9 kJ/mol @ 25°C (sol)	[10],[105]
	64.23 @ 25°C (gas)	[10],[105]

Analytical chemistry:  $pP_{oct}$  = unknown  
 $pK_s$  = unknown  
 $pK_a$  = unknown  
 $pK_{BH}$  = unknown  
 Henry's law constant = unknown  
 Hydrolysis half-life = unknown

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

Solubility: Slightly soluble in alcohol, methanol, glycerin. Very soluble in water. [10],[105]

71.6 wt% in water @ 20°C	[32]
50. wt% in cold water	[105],[10]
100. wt% in hot water	[105]
122.2 wt% in water @ 103.3°C	[47]
0.88g/100cc @ 19.5°C in ethanol	[105]
4.91g/100cc @ 19.5°C in methanol	[105]

Form: White, granular powder or fused solid pieces with a faint almond odor. Commercial preparations are 95% pure. [56],[108]

Use: It is primarily used in the extraction of ores. Electroplating; nitriding, tempering and case hardening of steel; various manufacturing processes. [56],[32]

Fire and explosion hazard: Very low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable solid but can reduce to highly flammable HCN in the presence of air and moisture. Also can react explosively and cause fires with certain other chemicals. Emits toxic fumes of hydrogen cyanide, carbon monoxide and carbon dioxide, and nitrogen oxides when heated to decomposition. Fight fire with alcohol or polymer foam. Do not use CO<sub>2</sub> extinguisher on this material. WARNING -- fire fighting hazard: water spray can be used to fight fire in area containing potassium cyanide and to cool fire-exposed metal containers. However, direct contact of material with water or steam will cause decomposition liberating highly toxic hydrogen cyanide gas as well as generating a highly hazardous solution of dissolved cyanide which must be kept out of sewers and watercourses. potassium cyanide has been found to form explosive mixtures sometimes spontaneously with chlorates, nitrates and nitrogen trichloride plus ammonia. [107],[55]

Incompatibility: Strong oxidizers such as nitrates, chlorates, acids, acid salts; alkaloids; iodine; metallic salts; permanganates; chloral hydrate; and peroxides. Absorbs CO<sub>2</sub> from air. [56],[108],[55]

## 420 - Potassium Cyanide

**Handling:** Prevent contact with air or moisture. Do not breath vapor or dust (appropriate respirator or self-contained breathing apparatus). Prevent possibility of skin or eye contact (chemical protective suit, gloves, safety goggles or face shield). Readily absorbed through skin. Remove nonimpervious clothing immediately if wet or contaminated. Use only in well-ventilated area (fume hood). Provide emergency showers and eyewash stations. Keep container tightly closed and protected from light. Store in cool, dry, secure poison area. Air and moisture sensitive. [56],[107],[108],[32],[55]

**Health effects:** Potassium cyanide is a violent poison. Routes of entry are inhalation, skin absorption, ingestion, and eye and skin contact. Points of attack include the liver, kidneys, skin, cardiovascular system, and central nervous system. Symptoms include weakness, headaches, confusion, nausea, vomiting, eye, skin and lung irritation, slow gasping respiration, and cyanosis. [56],[108],[32],[55],[68]

**Toxicity:** High

TWA: 1.88 ppm (5 mg/m<sup>3</sup>) (skin) [1]  
STEL: no value set [1]  
CL: unknown  
IDLH: 18 ppm (50 mg/m<sup>3</sup>) [107]  
Peak: unknown  
Odor threshold: NA [107]  
Carcinogenicity: unknown  
Mutagenicity: unknown

**Exposure:**

External:

Non-lethal: unknown  
Lethal: unknown

Oral:

Non-lethal: 8.4 mg/day in water, max. allow. daily intake [56]  
Lethal: 2.9 mg/kg body wt -- death of an adult male [32]

Inhalation:

Short-term Inhalation Limit: 45-54 ppm (120-145 mg/m<sup>3</sup>) for .5-1 hr [32]  
Non-lethal: unknown  
Lethal: unknown

## Quinoline

C<sub>9</sub>H<sub>7</sub>N

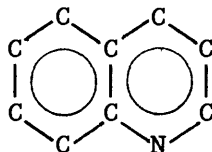
CAS RN: 91-22-5

Syn: Quinoline \* 1-Azanaphthalene \* B-500 \* 1-Benzanine \* 1-Benzazine \* 1-Benzine \* Benzo(*b*)pyridine \* Benzopyridine \* Chinoleine \* Chinoline \* Leucol \* Leucoline \* Leukol \* Quinolin \* UN 2656 (DOT) \* USAF EK-218 \*

Molecular formula: C<sub>9</sub>H<sub>7</sub>N

Aromatic Hydrocarbon

Structural formula:



## Physical properties:

Relative molecular mass:	129.16128	
Specific gravity:	1.095	[47], [10], [107], [104]
	1.093	[48]
	1.0929	[105], [106]
	1.09	[51], [108]
	1.0899	[22]
Boiling point:	242.°C	[48]
	238.05°C	[105]
	238.°C	[106], [56], [22]
	237.7°C	[51], [104], [108]
	237.1°C	[49], [47], [10]
	237.°C	[10], [107]
Melting point:	-14.5°C	[51]
	-14.85°C	[49]
	-14.9°C	[10]
	-15.°C	[47], [107], [22], [108]
	-15.6°C	[105], [106]
	-19.5°C	[104], [48]
Refractive index:	1.6268	[106], [105]
	1.62683	[108]
	1.6273	[10], [49]
Vapor pressure:	0.0112 kPa @ 25.16°C (0.084mm)	[49]
	0.1333 @ 59.7°C (1mm)	[105], [104]
Vapor density:	4.45	[51], [104]
	4.5	[107]
Evaporation rate:	unknown	
Relative dielectric permittivity:	9.559 @ 18°C	[2]
	9.12 @ 20°C (3 MHz)	[2]
	9.00 @ 25°C	[105], [10], [11]
	8.95 @ 25°C	[49], [2]
	5.05 @ 238°C	[105]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	0.66 MOhm-m @ 0°C	[11]
	0.45 @ 25°C	[10], [11]
	0.14 @ 50°C	[11]

## 422 - Quinoline

Critical temperature:	521.3°C	[49]
	520.0°C	[47]
	508.8°C	[105]
	509.°C	[10], [107]
Critical pressure:	5.8 MPa	[49]
Dynamic viscosity:	4.354 mPa-s @ 15°C	[10]
	3.145 @ 25°C	[49]
	2.997 @ 30°C	[49]
Kinematic viscosity:	3.984 $\mu\text{m}^2/\text{s}$ @ 15°C	
	2.878 @ 25°C	
	2.742 @ 30°C	
Surface tension:	45.65 mN/m @ 20°C	[49]
	45.0 @ 20°C (air)	[105], [107]
	44.82 @ 30°C	[49]
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	6.7 $\mu\text{m}^2/\text{s}$ (calc)	[59]
Solution diffusivity:	0.7 $\text{nm}^2/\text{s}$ (calc)	[59]
Electric dipole moment:	7.64x10 <sup>-30</sup> C-m	[105]
	7.27x10 <sup>-30</sup>	[10]
Ionization potential:	unknown	
Magnetic volume susceptibility:	-9.16x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	10.79 kJ/mol	[49]
	10.798	[105]
	10.82	[48]
Heat of vaporization:	49.71 kJ/mol	[49]
	52.65	[51], [105]
Heat of sublimation:	NA	
Heat capacity @ 25°C:	0.1992 kJ/(mol-K) (liq)	[105]
Heat of combustion:	-4700.72 kJ/mol @ 25°C (liq)	[49]
	-4703.87 @ 20°C (liq)	[105]
Heat of formation:	156.3 kJ/mol @ 25°C (liq)	[10]
Gibbs (free) energy:	275.9 kJ/mol @ 25°C (liq)	[10]
Analytical chemistry: pP <sub>oct</sub> =	2.06	[21]
	2.03	[59]
	2.02	[21]
pK <sub>s</sub> =	unknown	
pK <sub>a</sub> =	9.2 @ 20°C	[11]
	9.5	[108]
pK <sub>BH</sub> =	4.80 @ 20°C in water	[10], [105]
	4.94 @ 25°C in aqueous ethanol	[49]
Henry's law constant =	0.0021 dimensionless (calc)	[59]
Hydrolysis half-life =	unknown	

**Electrochemical data:** Cover and Folliard (1971), Folliard and Cover (1971), Fujinaga et al. (1966), Wiberg and Lewis (1970)

**Clay-organic interaction data:** Doehler and Young (1962), Greene-Kelly (1955), Helmy et al. (1983), Kutilek and Slangerova (1966), Yamamoto et al. (1969)

**Solubility:** Soluble in water. Miscible with ethanol, ether, acetone, benzene, carbon disulfide. Dissolves sulfur, phosphorus, arsenic trioxide. [51],[105],[10],[47],[104]

0.6 wt% in water [10]

6.0 vol% in water @ 25°C [47]

**Form:** Refractive, clear to light yellow-brown liquid. Penetrating, peculiar odor not as offensive as pyridine. Hygroscopic, absorbs as much as 22% water. Darkens on storage in ordinary, stoppered bottles. Volatile with steam. Weak base (neutral to phenolphthalein). Forms water soluble salts with strong acids. [51],[108],[107]

**Use:** Manufacture of dyes; preparation of hydroxyquinoline sulfate (niacin); as preservative for anatomical specimens; solvent for resins, terpenes. [108]

**Fire and explosion hazard:** Low.

Flash point: (CC) 107.2°C [107]

uel: unknown

lel: unknown

Autoign. temp.: 480°C [51],[107],[22]

Slightly flammable liquid. Slight fire hazard when exposed to heat.

Dangerous when heated to decomposition as it emits toxic fumes of nitrogen oxides, CO, and CO<sub>2</sub>. Fight fire with water, dry chemical powder, alcohol or polymer foam, CO<sub>2</sub>. [51],[107],[55]

**Incompatibility:** Strong oxidizing agents; strong acids; dinitrogen tetroxide; linseed oil; thionyl chloride; maleic anhydride; perchromates. May attack some forms of plastics. [51]

**Handling:** Avoid moisture, light and heat. Do not breath mist or vapor (appropriate respirator or self-contained breathing apparatus recommended). Do not get in eyes, on skin or on clothing (rubber gloves; lab coat and apron; goggles and shield). Use in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Keep product out of light. Store in cool, dry, secure poison area. [57],[56],[107]

**Health effects:** Quinoline is an irritant and potential carcinogen. Route of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include nervous system, liver, kidneys, respiratory system, eyes, and skin. It is irritating to eyes, skin, mucous membranes, and upper respiratory tract. Inhalation may cause headaches, dizziness and nausea. Contact with eyes and skin causes irritation. Potential to induce liver carcinoma. Laboratory experiments have shown chronic overexposure may lead to mutagenic effects. The chemical, physical, and toxicological properties have not been thoroughly investigated. [56],[55]

## 424 - Quinoline

### Toxicity: Unknown

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: 71 ppm (375 mg/m<sup>3</sup>) [107]

0.016-4.3 ppm (0.08-23 mg/m<sup>3</sup>) [104]

Carcinogenicity: animal positive [56]

Mutagenicity: experimental neoplastic effects [51]

equivalent tumorigenic agent [51]

positive test response [37]

### Exposure: Unknown

#### External:

Non-lethal: unknown

Lethal: unknown

#### Oral:

Non-lethal: unknown

Lethal: unknown

#### Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown



## Selenium

## Se

CAS RN: 7782-49-2

Syn: Selenium \* Se \* C.I. 77805 \* Colloidal selenium \* Elemental selenium  
 \* Non-pyrophoric selenium metal powder \* Selen (polish) \* Selenate \*  
 Selenium alloy \* Selenium base \* Selenium dust \* Selenium Homopolymer \* UN  
 2658 (DOT) \* Vandex \*

Molecular formula: Se

Element

## Physical properties:

Relative molecular mass:	78.96	
Specific gravity:	4.26-4.81	[51],[47]
	4.28-4.81	[108]
	4.45-4.8	[32]
	4.48-4.81	[10]
	4.81	[105]
	4.400	[48]
Boiling point:	690.°C	[51]
	688.°C	[47],[48]
	685.°C	[108],[22],[32],[10]
	684.9°C	[47]
	683.9°-685.9°C	[105]
Melting point:	220.°C	[48]
	217.°C	[108],[22],[47],[105]
	170.°-221°C	[10]
	170.°-217°C	[51]
	150.°C	[32]
Refractive index:	2.92 amorphous solid	[105]
	3.00	[105]
	4.04	[105]
Vapor pressure:	<0.000133 kPa @ 20°C (0.001mm)	[32]
	0.133 @ 356°C (1mm)	[51],[105]
Vapor density:	unknown	
Evaporation rate:	unknown	
Relative dielectric permittivity:	6.6 @ 17°-22°C	[105]
	5.4 @ 250°C	[20]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.428 W/(m-K) @ 0°C	[105]
	0.519 @ 25°C	[105]
Electrical resistivity:	1.x10 <sup>6</sup> MOhm-m @ 0°C	[105]
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	95.0 mN/m @ 220°C in vacuum	[105]
	92.4 @ 217°C	[20]
	92.5 @ 217°C	[108]
	88.0 @ 230°-250°C	[105]
Contact angle:	NA	
Thermal expansion coefficient:	0.000037 K <sup>-1</sup> @ 20°C	[48],[108]
Compressibility:	NA	
Vapor diffusivity:	NA	
Solution diffusivity:	NA	

## 426 - Selenium

Electric dipole moment:	unknown	
Ionization potential:	9.75 eV (VUS)	[105]
Magnetic volume susceptibility:	-314.x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	5.11 kJ/mol	[105]
	5.42	[108],[48]
	5.44	[10]
Heat of vaporization:	85.9533 kJ/mol	[48]
	86.25	[108]
Heat of sublimation:	NA	
Heat capacity @ 25°C:	0.0254 kJ/(mol-K) (sol-black)	[10]
	0.02084 (gas)	[10]
Heat of combustion:	NA	
Heat of formation:	0. kJ/mol @ 25°C (sol-black)	[105],[10]
	6.7 (sol-red)	[10]
	202.52 (gas)	[105]
	227.2 (gas)	[10]
Gibbs (free) energy:	0. kJ/mol @ 25°C (sol-black)	[105],[10]
	162.32 (gas)	[105]
	187.19 (gas)	[10]

Analytical chemistry:	pP <sub>oct</sub> =	NA
	pK <sub>s</sub> =	NA
	pK <sub>a</sub> =	NA
	pK <sub>BH</sub> =	NA
	Henry's law constant =	NA
	Hydrolysis half-life =	NA

Electrochemical data: Zhdanov (1975)

Clay-organic interaction data: inorganic

Solubility: Insoluble in cold or hot water. Soluble in H<sub>2</sub>SO<sub>4</sub>, CHCl<sub>3</sub>, HNO<sub>3</sub>, H<sub>2</sub>SO<sub>4</sub>, CS<sub>2</sub>, benzene. [32],[47],[105]

Form: A metal which exists in three forms. A red amorphous powder which becomes a steel grey form on standing, and crystalline red on heating. It is a non-metallic, odorless element. Selenium is found in the sludges and sediments from electrolytic copper refining. Elemental selenium does not appear in nature but is found in the rare minerals crooksite and clausthalite. It has atomic number 34 (Group VIA) with valence states of -2, +4, and +6. [51],[32],[56],[22]

Use: Used in selenium rectifiers, in the production of photocells and exposure meters for photographic use, as a vulcanizing agent for rubber, to convert a.c. electricity to d.c., for reproducing and copying documents, as a glass decolorizer, as a photographic toner, as an additive to stainless steel, as an insecticide, in semiconductor fusion experiments, in the manufacture of electrodes, in antidandruff shampoos, in cancer chemotherapy. [105],[56],[90]

**Fire and explosion hazard:** Very low.

Flash point: NA

UEL: NA

LEL: NA

Autoign. temp.: NA

Nonflammable solid. When heated to decomposition it emits toxic fumes.

Use extinguishing media appropriate to surrounding fire conditions.

[51],[32],[55]

**Incompatibility:** Barium carbide; bromine pentafluoride; calcium carbide; chlorates; chlorine trifluoride; chromic oxide ( $\text{CrO}_3$ ); fluorine; lithium carbide; lithium silicon ( $\text{Li}_6\text{Si}_2$ ); nickel; nitric acid; sodium; nitrogen trichloride; oxygen; potassium; potassium bromate; rubidium carbide; zinc; silver bromate; strontium; carbide; thorium carbide; uranium. Contact of selenium with acids may cause formation of poisonous hydrogen selenide gas. Contact of selenium with strong oxidizing agents may cause fires and explosions. [32],[51],[56],[55]

**Handling:** Do not breathe vapor (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (chemical resistant gloves and suit; safety goggles or face shield). Readily absorbed through skin. Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [55],[56],[57]

**Health effects:** Elemental selenium is considered to be relatively nonirritating and is poorly absorbed. However, hydrogen selenide and other selenium compounds are extremely toxic, and resemble arsenic in their physiological reactions. Routes of entry are inhalation, ingestion, percutaneous absorption of liquid, and eye and skin contact. Points of attack include respiratory system, skin, eyes, and gastrointestinal tract. Compounds can be irritating to the eyes, upper respiratory tract, and skin. Prolonged exposure may cause paleness, coated tongue, stomach disorders, nervousness, metallic taste and a garlic odor breath. There is strong evidence that selenium is an essential trace element for man. In controlled doses it reduces chemotherapy side effects. [32],[56],[105],[55],[90]

**Toxicity:** Very low.

TWA: 0.06 ppm (0.2 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: 31 ppm (100 mg/m<sup>3</sup>) [56]

Peak: unknown

Odor threshold: odorless [32]

Carcinogenicity: may be anticarcinogenic [90]

Mutagenicity: experimental equivocal tumorigenic agent [51]  
equivocal tumorigenic agent by RTECS criteria [55]

**Exposure:** Unknown

## 428 - Silver

Silver

Ag

CAS RN: 7440-22-4

Syn: Silver \* Ag \* Argentum \* C.I. 77820 \* L 3 \* Shell silver \* Silflake  
135 \* Silver atom \* Silver metal \* Sr 999 \* V 9 \*

Molecular formula: Ag

Element

## Physical properties:

Relative molecular mass:	107.8682	[105]
Specific gravity:	10.4	[32]
	10.5	[47], [51], [48]
	10.50	[105]
	10.53	[22]
Boiling point:	1950.°C	[47], [48]
	2000.°C	[108]
	2164.°C	[10]
	2200.°C	[32]
	2212.°C	[22], [105], [51]
Melting point:	960.15°C	[10]
	960.5°C	[108], [47], [48]
	961.°C	[22]
	961.93°C	[105], [51]
	966.°C	[32]
Refractive index:	0.54	[105]
Vapor pressure:	essentially 0. kPa @ 20°C	[32]
	0.133 @ 1357°C (1mm)	[105], [47]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	NA	
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	410.539 W(m-K) @ 0°C	[48]
	428. @ 0°C	[20]
	429. @ 0°C	[105]
	429. @ 25°C	[105]
	391.931 @ 100°C	[48]
	426. @ 100°C	[105]
Electrical resistivity:	1.467x10 <sup>-14</sup> MOhm-m @ 0°C	[105]
	1.587x10 <sup>-14</sup> @ 20°C	[105]
	1.6x10 <sup>-14</sup> @ 22°C	[105]
Critical temperature:	7226.9°C	[20]
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	727. mN/m @ 961°C in helium	[105]
	800. @ 970°C	[20]
	850. @ 970°C	[20]
	908. @ 1000°C	[105]
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	NA	

Ionization potential:	7.574 eV (VUS)	[105]
Magnetic volume susceptibility:	-245.x10 <sup>-6</sup> SI units @ 23.8°C	[105]
Speed of sound:	3650. m/s long. wave in bulk	[105]
	1610. shear wave in bulk	[105]
	2680. long. wave in thin rod	[105]
Heat of melting:	11.29 kJ/mol	[48]
	11.30	[105], [47]
	11.95	[10]
Heat of vaporization:	234.84 kJ/mol	[48]
	254.22	[47]
	258.24	[10]
Heat of sublimation:	NA	
Heat capacity @ 25°C:	0.0254 (sol)	[10]
	0.0255 (sol)	[105]
	0.0218 kJ/(mol-k) (liq-Ag <sup>+</sup> )	[10]
	0.0208 (gas)	[10]
Heat of combustion:	NA	
Heat of formation:	0. kJ/mol @ 25°C (sol)	[10], [105], [47]
	105.6 (liq-Ag <sup>+</sup> )	[10]
	106.0 (liq-Ag <sup>+</sup> )	[105]
	284.7 (gas)	[10]
	289.4 C (gas)	[105]
Gibbs (free) energy:	0. kJ/mol @ 25°C (sol)	[10], [105], [47]
	77.16 (liq-Ag <sup>+</sup> )	[105], [10]
	245.8 (gas)	[10]
	250.5 (gas)	[105]
Analytical chemistry:	pP <sub>oct</sub> = NA	
	pK <sub>s</sub> = NA	
	pK <sub>a</sub> = >11.1 (Ag <sup>+</sup> )	[10]
	pK <sub>BH</sub> = NA	
	Henry's law constant = NA	
	Hydrolysis half-life = NA	

**Electrochemical data:** Shumilova and Zhutaeva (1978)

**Clay-organic interaction data:** inorganic

**Solubility:** Insoluble in hot and cold water. Corrodes in HNO<sub>3</sub>, hot sulfuric and hot nitric acids. [105], [22], [32], [47], [56]

**Form:** Soft, ductile, malleable, lustrous, white metal with no odor. It has atomic number 47 (Group IB) and valence state of +1. Highest electrical and thermal conductivity of all metals. Resists oxidation, but tarnishes in air through reaction with atmospheric sulfur compounds. [51], [22]

## 430 - Silver

**Use:** Silver may be alloyed with copper, aluminum, cadmium, lead, or antimony. The alloys are used in the manufacture of silverware, jewelry, coins, ornaments, plates, commutators, scientific instruments, automobile bearings, and grids in storage batteries. It is also used in chrome-nickel steels, in solders and brazing alloys, in the application of metallic films on glass and ceramics, to increase corrosion resistance to sulfuric acid, in photographic films, plates and paper, as an electroplated undercoating for nickel and chrome, as a bactericide for sterilizing water, fruit juices, vinegar, etc., in bus bars and windings in electrical plants, in dental amalgams, and as a chemical catalyst in the synthesis of aldehydes. Because of its resistance to acetic and other food acids, it is utilized in the manufacture of pipes, valves, vats, pasteurizing coils and nozzles for the milk, vinegar, cider, brewing, and acetate rayon silk industries. [56]

**Fire and explosion hazard:** Very low.

Flash point: NA

UEL: NA

LEL: NA

Autoign. temp.: NA

Nonflammable solid. Moderate fire hazard in the form of dust, when exposed to flame. [51]

**Incompatibility:** Contact of silver and soluble silver compounds with acetylene may cause the formation of silver acetylide that is sensitive to shock. Contact with ammonia may cause formation of compounds that are explosive when dry. Contact with strong hydrogen peroxide solutions will cause violent decomposition to oxygen gas. [32]

**Handling:** Keep away from heat and open flame when in the form of dust. Do not breathe dust or fume (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (chemical resistant gloves and suit; safety goggles or face shield). Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [55],[56],[57]

**Health effects:** Silver can be toxic. Routes of entry are inhalation of fumes or dust, ingestion of solutions or dust, and eye and skin contact. Points of attack include respiratory system (particularly the nasal septum), skin, and eyes. Can cause discoloration or blue-gray darkening of the eyes, nose, throat, and skin. Once deposited in the body it is poorly excreted in the urine. [32]

**Toxicity:** Low.

TWA: 0.0023 ppm (0.01 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: unknown

Mutagenicity: unknown

**Exposure:**

External:

Non-lethal: 0.23 ppm (1 mg/m<sup>3</sup>) -- toxic effects on the skin [51]

Lethal: unknown

Oral:

Non-lethal: 1 to 5 g -- generalized argyria [32]

0.9 g -- visible argyria [56]

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown

## 432 - Sodium Cyanide

Sodium Cyanide

NaCN

CAS RN: 143-33-9

Syn: Sodium cyanide \* Cyanide of sodium \* Cyanogran \* Cymag \* Hydrocyanic acid \* Hydrocyanic acid, sodium salt \* Sodium salt \* RCRA Waste Number P106 \* UN 1689 (DOT) \*

Molecular formula: NaCN

Cyanide

## Physical properties:

Relative molecular mass:	49.01	
Specific gravity:	1.60 @ 25°C	[32],[107]
Boiling point:	1530.°C	[10]
	1500.°C	[32]
	1496.°C	[105],[51]
Melting point:	563.°C	[22],[108]
	563.7°C	[105],[51]
	562.°C	[10]
	560.°C	[32]
Refractive index:	1.452	[105],[10]
Vapor pressure:	0. kPa @ 20°C	[32]
Vapor density:	NA	[32],[107]
Evaporation rate:	NA	[32]
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	NA	[107]
Critical pressure:	NA	[107]
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	[107]
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	17. kJ/mol	[20]
	18.25	[105],[107]
	8.79	[10]
Heat of vaporization:	155. kJ/mol @ 760mm	[20]
	148.2	[10]
Heat of sublimation:	172.9 kJ/mol	[10]
Heat capacity @ 25°C:	0.0687 kJ/(mol-K) (sol)	[10]
	0.0502 (gas)	[10]
Heat of combustion:	NA	[107]
Heat of formation:	-87.55 kJ/mol @ 25°C (sol)	[10],[105]
	-94.08 @ 25°C (sol)	[57]
	94.33 @ 25°C (gas)	[10],[105]



Gibbs (free) energy:                    -76.49 kJ/mol @ 25°C (sol)            [10],[105]  
    67.37                    @ 25°C (gas)            [10],[105]

Analytical chemistry:  $pP_{oct}$  =            0.44 (est)                                    [91]  
     $pK_s$  =    unknown  
     $pK_a$  =    unknown  
     $pK_{BH}$  = unknown  
                                  Henry's law constant = unknown  
                                  Hydrolysis half-life = unknown

Electrochemical data: Unknown

Clay-organic interaction data: [8]

Solubility: Soluble in alcohol and ammonia. Very soluble in water. Water solution is strongly alkaline and rapidly decomposes. [22],[108]

48. wt% in water @ 10°C                    [105]

58. wt% in water @ 20°C                    [32]

58.7 wt% in water @ 20°C                    [10]

82. wt% in water @ 35°C                    [105]

Form: White granules or fused pieces (solid). Odorless when dry. Somewhat deliquescent in damp air and emits slight odor of bitter almonds. [108]

Use: Solution readily "dissolves" gold and silver in presence of air. Used in ore extraction, electroplating baths, case hardening of steel, fumigating, and manufacturing of dyes, pigments, chelating compounds, and other cyanides. [108],[56],[22]

Fire and explosion hazard: Very low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable solid but can reduce to highly flammable HCN in presence of air and water. Can react explosively and cause fires with certain other chemicals. Emits toxic gases of hydrogen cyanide, carbon monoxide and carbon dioxide, nitrogen oxides when heated to decomposition. Fight fire with alcohol or polymer foam. Do not use CO<sub>2</sub> extinguisher on this material. [107],[55]

Incompatibility: Strong oxidizers such as nitrates and chlorates; acids and acid salts. [32],[56],[51]

Handling: Avoid contact with air or moisture. Do not breathe dust (appropriate respirator or self-contained breathing apparatus). Prevent possibility of skin and eye contact (chemical protective suit, gloves, safety goggles or and face shield). Readily absorbed through skin. Remove nonimpervious clothing immediately if wet or contaminated. Provide emergency showers and eyewash stations. Keep container tightly closed. Store in dry, cool, secure poison area. [56],[107],[108],[55]

#### 434 - Sodium Cyanide

**Health effects:** Sodium cyanide is a violent poison. Routes of entry are inhalation, skin absorption, ingestion, and eye and skin contact. Points of attack include liver, kidneys, skin, cardiovascular system, and central nervous system. Symptoms include weakness, headaches, confusion, nausea, vomiting, eye, skin and lung irritation, slow gasping respiration, and cyanosis. [56],[32],[55],[68],[91]

**Toxicity:** High

TWA: 2.49 ppm (5 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 24.9 ppm (50 mg/m<sup>3</sup>) [107]

Peak: unknown

Odor threshold: NA [107]

Carcinogenicity: unknown

Mutagenicity: indefinite [91]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: 8.4 mg/day in water, max. allow. daily intake [56]

Lethal: 180 mg [107]

2.2 mg/kg body wt -- death of an adult male [32],[51]

2.857 mg/kg body wt -- death of an adult human [32],[51]

6.557 mg/kg -- adult male [55]

Inhalation:

Short-term Inhalation Limit: 45-54 ppm for 1/2 to 1 hr [32]

Non-lethal: unknown

Lethal: unknown

1,1,2,2-Tetrachloroethane

 $C_2H_2Cl_4$ 

CAS RN: 79-34-5

Syn: 1,1,2,2-Tetrachloroethane \* Ethane, 1,1,2,2-tetrachloro- \* Acetylene  
 tetrachloride \* Bonoform \* Cellon \* 1,1-Dichloro-2,2-dichloroethane \*  
 Ethane tetrachloride \* NCI-C03554 \* RCRA Waste Number U209 \* TCE \*  
 Tetrachlorethane \* Tetrachloroethane \* sym-Tetrachloroethane \* UN 1702  
 (DOT) \* Westron \*

Molecular formula:  $Cl_2CHCHCl_2$ 

Polychlorinated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	167.85		
Specific gravity:	1.600	[104], [47], [51], [32]	
	1.5953		[105], [16]
	1.595		[107]
	1.59449		[49]
Boiling point:	146.5°C		[22], [108]
	146.4°C		[104], [51]
	146.3°C		[10], [47], [107]
	146.2°C		[105], [16]
	146.°C		[56], [32]
	145.1°C		[49]
Melting point:	-36.°C		[47], [105], [10]
	-43.8°C (fp)	[10], [49], [104], [105], [107]	
	-43.°C		[22]
	-42.5°C		[104], [32]
	-44.°C		[108]
Refractive index:	1.4940		[49], [105], [16]
	1.49419		
Vapor pressure:	0.133 kPa @ -3.8°C	(1mm)	[105], [47]
	0.666 @ 20°C	(5mm)	[104]
	0.666 @ 20.7°C	(5mm)	[47]
	0.793 @ 25°C	(5.95mm)	[16], [49]
	1.133 @ 30°C	(8.5mm)	[104]
	1.333 @ 33°C	(10mm)	[105], [47]
	5.333 @ 60.8°C	(40mm)	[105]
Vapor density:	5.79		[104], [107]
	5.8		[32]
Evaporation rate:	0.65		[32]
Relative dielectric permittivity:	8.20 @ 20°C		[10], [11]
	8.50 @ 20°C (1.8 MHz)		[2]
Loss tangent:	unknown		
Relaxation time:	unknown		
Thermal conductivity:	0.114 W/(m-K) @ 20°C		[105]
Electrical resistivity:	(not measurable)		[49]
Critical temperature:	388.0°C		[10]
Critical pressure:	unknown		
Dynamic viscosity:	2.66 mPa-s @ 0°C		[48]
	2.15 @ 10°C		[48]
	1.844 @ 15°C		[105], [10]
	1.75 @ 20°C		[48]
	1.48 @ 30°C		[48]
	1.28 @ 40°C		[48]

# 436 - 1,1,2,2-Tetrachloroethane

Kinematic viscosity:	1.66 $\mu\text{m}^2/\text{s}$ @ 0°C	
	1.34 @ 10°C	
	1.151 @ 15°C	
	1.09 @ 20°C	
	0.93 @ 30°C	
	0.80 @ 40°C	
Surface tension:	37.85 mN/m @ 20°C	[107], [16]
	36.04 @ 20°C	[49]
	36.03 @ 22.5°C (air)	[105]
	36.41 @ 30°C	[16]
	35.00 @ 40°C	[16]
	33.30 @ 40°C	[49]
Contact angle:	unknown	
Thermal expansion coefficient:	0.000998 $\text{K}^{-1}$	[49]
Compressibility:	0.617 $\text{nPa}^{-1}$ @ 25°C	[105]
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	4.403x10 <sup>-30</sup> C-m	[105], [10]
	5.704x10 <sup>-30</sup>	[49]
Ionization potential:	11.10 eV (EI)	[105]
Magnetic volume susceptibility:	-10.76x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	41.521 kJ/mol	[105]
	38.69	[10]
	38.64	[49]
	38.61	[107]
	36.20	[16]
Heat of sublimation:	44.80 kJ/mol	[10]
Heat capacity @ 25°C:	0.1657 kJ/ (mol-K) (liq)	[49]
	0.1658 (liq)	[10]
	0.1009 (gas)	[10]
Heat of combustion:	-971.19 kJ/mol @ 18°C (liq)	[49]
Heat of formation:	223.20 kJ/mol @ 25°C (liq)	[10]
	-196.6 (liq)	[49], [10]
	-149.0 (gas)	[49]
	-152.8 (gas)	[10]
Gibbs (free) energy:	-95.04 kJ/mol @ 25°C (liq)	[10]
	-85.62 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	2.56	[8], [41]
	2.39	[4], [27], [31], [24]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	0.039 kPa-m <sup>3</sup> /mol	[41]
	0.0461 @ 25°C (calc)	[24]
	0.0462 @ 25°C	[41]
	0.0072 @ 37°C	[41]
Hydrolysis half-life =	7.9x10 <sup>6</sup> to 1.3x10 <sup>8</sup> sec	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Karickhoff (1981), Rao et al. (1988).

**Solubility:** Almost insoluble in water. Soluble in acetone, benzene, chloroform. Miscible with methanol, ethanol, ether, petroleum ether, carbon tetrachloride, carbon disulfide, dimethylformamide, oils. Has the highest solvent power of the chlorinated hydrocarbons.

[108],[104],[10],[108]

0.29 wt% in water @ 20°C [10],[47],[104]

0.287 wt% in water @ 20°C [49]

0.29 wt% in water @ 20°C [32]

0.286 wt% in water @ 25°C [108]

**Form:** Colorless to pale yellow or yellowish-green, heavy, mobile liquid. Mild, sweetish, suffocating chloroform-like odor similar to several other chlorinated hydrocarbons such as carbon tetrachloride.

[51],[108],[107],[41]

**Use:** Dry cleaning agent; soil fumigant; in cement; in lacquers; manufacture of tetrachloroethene, 1,1-dichloroethene, artificial silk, artificial leather, artificial pearls, paint, varnish, rust remover, bleach, insecticides; solvent for chromium chloride impregnated in furs, chlorinated rubber; in the estimation of water content in tobacco and many drugs; cleansing and degreasing metals; photo films, resins and waxes; herbicide; weed killer; denaturant for ethanol. [104],[56],[108],[41]

**Fire and explosion hazard:** Very low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable liquid but dangerous. Evolves spontaneous flammable gas when heated in contact with solid potassium hydroxide. Any water can cause appreciable hydrolysis even at room temperature. Both hydrolysis and oxidation become comparatively rapid above 110°C. Emits highly toxic decomposition products such as phosgene, hydrochloric acid, CO, CO<sub>2</sub>, or dichloroacetyl chloride. [51],[107],[55]

**Incompatibility:** Chemically active metals; strong oxidizing agents; strong caustics; hot iron; aluminum; zinc in presence of steam. Reacts violently with nitrates, 2,4-dinitrophenol disulfide, sodium, potassium.

[51],[32],[56],[55]

**Handling:** Avoid moisture. Prevent any possibility of inhalation (appropriate respirator or self-contained breathing apparatus). Prevent any possibility of contact of eyes, skin, or clothing (impervious clothing; rubber gloves; safety goggles, face shield). Readily absorbed through skin. Use with adequate ventilation (fume hood). Wash immediately with soap if skin is wet or contaminated. Remove impervious clothing immediately if wet or contaminated. Provide emergency showers and eyewash stations. Keep container tightly closed. Store in cool, dry, secure poison area or cabinet. [56],[57],[32],[107]

#### 438 - 1,1,2,2-Tetrachloroethane

**Health effects:** Routes of entry are inhalation, skin absorption, ingestion, and eye and skin contact. Points of attack include liver, kidneys, eyes, skin, and central nervous system. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. Liver and kidney damage may occur. If exposure is severe, within a few hours a deep dusky coloration of the skin may appear, followed by unconsciousness and death. Chronic exposure may cause fatigue, loss of appetite, tremors, weight loss, constipation, heart damage, blood changes, kidney damage, abdominal distress and pain, vomiting, dizziness, tenderness, and liver damage. [32],[56],[55],[93]

**Toxicity:** High.

TWA: 1 ppm (7 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 150 ppm (1030 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 0.5 ppm (3.4 mg/m<sup>3</sup>) [107]

<3 ppm (20 mg/m<sup>3</sup>) [104]

3 ppm (20 mg/m<sup>3</sup>) -- detectable odor [51]

3-5 ppm (20-34 mg/m<sup>3</sup>) [32]

7.3 ppm (50 mg/m<sup>3</sup>) -- detection [104]

Carcinogenicity: possible human; animal positive [51]

Mutagenicity: some positive evidence [93],[37]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: 30 mg/kg body wt -- CNS [51]

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: 10 ppm (70 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: 10 ppm (70 mg/m<sup>3</sup>) -- unsatisfactory [104]

20 ppm (135 mg/m<sup>3</sup>) -- symptoms of illness [104]

20-65 ppm -- nausea, vomiting, and abdominal pain [32]

50 ppm (345 mg/m<sup>3</sup>) -- severe toxic effects [104]

145 ppm (1000 mg/m<sup>3</sup>) for 30 min -- CNS [51]

335 ppm (2300 mg/m<sup>3</sup>) for 10 min or 186 ppm (1275 mg/m<sup>3</sup>)  
for 30 min -- upper respiratory irritation and central  
nervous system effects [32]

Lethal: unknown

Tetrachloroethene

 $C_2Cl_4$ 

CAS RN: 127-18-4

Syn: Tetrachloroethene \* Ethene, tetrachloro- \* Ankilostin \* Antisol 1 \* Carbon bichloride \* Carbon dichloride \* Dee-Solv \* Didakene \* Dow-per \* ENT 1860 \* Ethylene tetrachloride \* Fedal-UN \* NCI-C04580 \* Nema \* PCF \* PER \* Perawin \* PERC \* Perchlor \* Perchlorethylene \* Perchloroethylene \* Perclene \* Perclene D \* Percosolve \* Perk \* Perklone \* Persec \* RCRA Waste Number U210 \* Tetlen \* Tetracap \* Tetrachlorethylene \* Tetrachloroethylene \* 1,1,2,2-Tetrachloroethylene \* Tetraleno \* Tetralex \* Tetravec \* Tetroguer \* Tetropil \* UN 1897 (DOT) \*

Molecular formula:  $Cl_2C=CCl_2$ 

Polychlorinated Aliphatic Halide

## Physical properties:

Relative molecular mass:	165.834	
Specific gravity:	1.62	[32]
	1.62283	[49]
	1.6227	[105]
	1.62272	[15]
	1.626	[104]
	1.63	[107]
Boiling point:	1.6230	[10], [108]
	120.8°C	[47]
	120.97°C	[15]
	121.°C	[10], [22], [105], [108], [107]
	121.20°C	[51], [32]
	121.4°C	[104]
Melting point:	-19.°C	[105]
	-22.°C	[108]
	-22.35°C	[49]
	-22.4°C	[22], [32], [107], [10]
	-22.7°C	[104]
	-23.35°C	[51]
Refractive index:	1.5053	[15], [105]
	1.5055	[108]
	1.50576	[10], [49]
Vapor pressure:	0.133 kPa @ -20.6°C (1mm)	[105], [47]
	0.655 @ 2.4°C (5mm)	[47]
	1.333 @ 13.8°C (10mm)	[47], [105]
	1.87 @ 20°C (14mm)	[32], [104]
	2.106 @ 22°C (15.8mm)	[51]
	2.462 @ 25°C (18.47mm)	[49], [15]
	2.67 @ 26.6°C (20mm)	[47]
	3.20 @ 30°C (24mm)	[104]
	5.33 @ 40.1°C (40mm)	[105], [47]
		[51], [32], [104]
Vapor density:	5.83	
Evaporation rate:	2.10	[49]
	2.8	[32]
Relative dielectric permittivity:	2.276 @ -20°C	[2]
	2.280 @ 25°C	[49]
	2.30 @ 25°C	[11], [10]
	2.301 @ 30°C	[2]
Loss tangent:	unknown	
Relaxation time:	unknown	

#### 440 - Tetrachloroethene

Thermal conductivity:	unknown	
Electrical resistivity:	$1.801 \times 10^{-5}$ MOhm-m @ 20°C	[49]
Critical temperature:	347.°C	[107], [49]
	347.1°C	[10]
Critical pressure:	4.491 MPa	[49]
Dynamic viscosity:	1.162 mPa-s @ 0°C	[48]
	1.020 @ 10°C	[48]
	0.8916 @ 20°C	[15]
	0.897 @ 20°C	[48]
	0.816 @ 30°C	[48]
	0.7413 @ 40°C	[15]
	0.734 @ 40°C	[48]
Kinematic viscosity:	0.7164 $\mu\text{m}^2/\text{s}$ @ 0°C	
	0.6289 @ 10°C	
	0.54976 @ 20°C	
	0.5530 @ 20°C	
	0.5031 @ 30°C	
	0.45702 @ 40°C	
	0.4525 @ 40°C	
Surface tension:	32.86 mN/m @ 15°C	[49], [10]
	31.74 @ 20°C (vapor)	[105]
	31.33 @ 20°C	[15]
	31.3 @ 20°C	[107]
	31.30 @ 25°C	[49]
	31.27 @ 30°C	[10]
	30.81 @ 30°C	[15]
	30.20 @ 40°C	[15]
Contact angle:	unknown	
Thermal expansion coefficient:	0.00102 K <sup>-1</sup> @ 0-25°C	[49]
Compressibility:	unknown	
Vapor diffusivity:	8.0 $\mu\text{m}^2/\text{s}$	[59]
Solution diffusivity:	0.75 nm <sup>2</sup> /s (calc)	[59]
Electric dipole moment:	0. C-m	[10], [49]
Ionization potential:	9.32 eV (PI)	[105]
Magnetic volume susceptibility:	$-10.08 \times 10^{-6}$ SI units @15°C	[105]
Speed of sound:	unknown	
Heat of melting:	10.47 kJ/mol	[10]
	10.56	[49]
Heat of vaporization:	34.78 kJ/mol	[107]
	34.75	[10]
	34.74	[47]
	34.72	[49], [15]
Heat of sublimation:	39.36 kJ/mol	[10]
Heat capacity @ 25°C:	0.0350 kJ/(mol-K) (liq)	[49]
	0.14411 (liq)	[105]
	0.0950 (gas)	[10], [105]
Heat of combustion:	-679.9 kJ/mol @ 25°C (liq)	[49]
Heat of formation:	-52.33 kJ/mol @ 25°C (liq)	[105], [49]
	-12.14 (gas)	[105], [49]
	-14.24 (gas)	[10]
Gibbs (free) energy:	4.60 kJ/mol @ 25°C (liq)	[105]
	20.52 (gas)	[10]
	22.61 (gas)	[105]



Analytical chemistry:	pP <sub>oct</sub> =	3.40	[24],[59]
		2.88	[8],[27],[31]
		2.60	[21]
		2.58	[4]
		2.10 - 2.88	[41]
	pK <sub>s</sub> =	NA	
	pK <sub>a</sub> =	NA	[31]
	pK <sub>BH</sub> =	NA	
Henry's law constant =		0.291 kPa·m <sup>3</sup> /mol	[41]
		1.55	[41]
		1.51	[24]
		1.33	[41]
		6.00 @ 37°C	[41]
Hydrolysis half-life =		0.82 dimensionless	[59]
		2.3x10 <sup>7</sup> sec	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Karickhoff (1981).

Solubility: Almost insoluble in water. Miscible with ethanol, ether, benzene, chloroform, alcohol, oils. [10],[108],[104],[32],[47]

0.015 wt% in water @ 20°C	[32]
0.02 wt% in water @ 20°C	[47]
0.015 wt% in water @ 25°C	[49],[104]

Form: Colorless liquid, chloroform-like odor. [51]

Use: Dry cleaning; degreasing metals; solvent for fats, greases, waxes, rubber, gums, caffeine from coffee; remove soot from industrial boilers; chemical intermediate; manufacture of paint removers, printing inks; fumigant; medically as an anthelmintic. [108],[56],[104]

Fire and explosion hazard: Very low.

Flash point: none [55]

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable liquid. When heated to decomposition, it emits highly toxic fumes of phosgene gas, hydrogen chloride gas, CO, and CO<sub>2</sub>. Use extinguishing media appropriate to surrounding fire conditions. [51],[108],[107],[55]

Incompatibility: Strong oxidizers; strong bases; barium; beryllium; lithium; N<sub>2</sub>O<sub>4</sub>; metals; sodium hydroxide. [51],[32],[56],[55]

## 442 - Tetrachloroethene

**Handling:** Avoid heat and flame. Do not breathe vapor or mist (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, on clothing (chemical resistant gloves; safety goggles; other protective clothing). Use with adequate ventilation (fume hood). Wash promptly if skin is wet or contaminated. Work clothing should be changed daily if it is possible or probable that clothing is contaminated. Remove nonimpervious clothing promptly if wet or contaminated. Safety shower and eye bath stations should be provided. Exposure to and/or consumption of alcohol may increase toxic effects. Keep container tightly closed. Store in a cool, dry, secure poison area. [56],[57],[55]

**Health effects:** Tetrachloroethene is an irritant with narcotic properties and a possible carcinogen. Routes of entry are inhalation, skin absorption, ingestion, and eye and skin contact. Points of attack include liver, kidneys, eyes, upper respiratory system, and central nervous system. Vapor or mist is irritating to the eyes, skin, mucous membranes, and upper respiratory tract. There may be vomiting, nausea, drowsiness, an attitude of irresponsibility, and even an appearance resembling alcoholic intoxication. This material also acts as an anesthetic, through the inhalation of excessive amounts within a short time. The symptoms of fatal intoxication are irritation to the eyes, nose and throat, then fullness in the head, mental confusion; there may be headache stupefaction, nausea and vomiting. Personnel suffering from subacute poisoning may suffer from such symptoms as headache, fatigue, nausea, vomiting, mental confusion and temporary blurring of the vision. This can occur when inadequate ventilation results in concentrations higher than 200 ppm. This material may also cause dermatitis. Chronic effects may include damage to the liver and kidneys. [51],[55],[94]

**Toxicity:** High.

TWA: 1 ppm (7 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: 10 ppm (68 mg/m<sup>3</sup>) for 15 min [51]

100 ppm (680 mg/m<sup>3</sup>) for 15 min (NIOSH) [32],[56]

200 ppm (1355 mg/m<sup>3</sup>) (OSHA) [32],[56]

IDLH: 500 ppm (3390 mg/m<sup>3</sup>) [107]

Peak: 300 ppm (2035 mg/m<sup>3</sup>) for 5 min [32]

Odor threshold: 5 ppm (34 mg/m<sup>3</sup>) [107]

50 ppm (340 mg/m<sup>3</sup>) [32],[56]

5-50 ppm (34-340 mg/m<sup>3</sup>) [104]

**Carcinogenicity:** possible human carcinogen [51]

animal positive (mouse-positive, rat-negative) [51],[40]

animal limited evidence [55]

carcinogenic by RTECS criteria [55]

positive in rats and mice [26]

**Mutagenicity:** neoplastic by RTECS criteria [55]

positive evidence [9]

nonmutagenic [37]

**Exposure:**

**External:**

Non-lethal: liquid on skin for 40 min -- severe burning, erythema [32]  
280 ppm (1900 mg/m<sup>3</sup>) for 2 hours -- eye irritation [51]

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: 0.5 to 5 g/kg body wt [107]

**Inhalation:**

Short-term Inhalation Limits: 100 ppm (680 mg/m<sup>3</sup>) for 60 min [107]

Non-lethal: 96 ppm (650 mg/m<sup>3</sup>) for 7 hr -- systemic effects [51]  
200 ppm -- lachrymation and burning of the eyes [32]  
513-690 ppm for 10 min -- nose and throat irritation [32]  
600 ppm for 10 min -- central nervous system effects [51]  
5000 ppm for 6 min -- vertigo, nausea, and confusion [32]

Lethal: 2857 mg/kg body wt -- death of an adult male [55]

## 444 - Thallium

Thallium

Tl

CAS RN: 7440-28-0

Syn: Thallium \* Tl \* Ramor \*

Molecular formula: Tl

Element

## Physical properties:

Relative molecular mass:	204.383	[105]
Specific gravity:	11.85	[10],[22],[47],[51],[105],[108]
Boiling point:	1457.°C	[51],[22],[108]
	1457.°C ± 10°C	[105]
	1487.°C	[10]
Melting point:	303.5°C	[10],[47],[51],[105],[108]
	302.°C	[22]
Refractive index:	NA	
Vapor pressure:	0.133 kPa @ 825°C (1mm)	[47],[51],[105]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	NA	
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	51.172 W/(m-K) @ 0°C	[48]
	46.9 @ 0°C	[105]
	46.1 @ 25°C	[105]
	44.3 @ 100°C	[105]
	41.868 @ 100°C	[48]
Electrical resistivity:	1.8x10 <sup>-13</sup> MOhm-m @ 0°C	[105]
	1.6x10 <sup>-13</sup> @ 22°C	[105]
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	464.5 mN/m @ 303°C	[105]
	450. @ 450°C	[105]
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	NA	
Ionization potential:	6.106 eV (VUS)	[105]
Magnetic volume susceptibility:	-639.6x10 <sup>-6</sup> SI units @ 25°C	[105]
Speed of sound:	unknown	
Heat of melting:	4.082 kJ/mol	[10]
	4.312	[105],[47],[108]
Heat of vaporization:	162.49 kJ/mol	[47]
	165.00	[10]
Heat of sublimation:	NA	
Heat capacity @ 25°C:	0.0263 kJ/(mol-K) (sol)	[10],[105]
	0.0208 (gas)	[10]
Heat of combustion:	NA	

Heat of formation:	0.	kJ/mol @ 25°C	(sol)	[10],[105],[47]
	5.78		(liq-Tl <sup>+</sup> )	[105]
	186.3		(gas)	[105]
	182.3		(gas)	[10]
Gibbs (free) energy:	0.	kJ/mol @ 25°C	(sol)	[10],[105],[47]
	-32.5		(liq-Tl <sup>+</sup> )	[105]
	151.6		(gas)	[105]
	147.54		(gas)	[10]

Analytical chemistry:	pP <sub>oct</sub> =	NA	
	pK <sub>s</sub> =	NA	
	pK <sub>a</sub> =	13.18 (Tl <sup>+</sup> )	[10]
	pK <sub>BH</sub> =	NA	
	Henry's law constant =	NA	
	Hydrolysis half-life =	NA	

Electrochemical data: Bellavance and Miller (1975)

Clay-organic interaction data: inorganic

Solubility: Insoluble in hot or cold water, but readily forms soluble compounds when exposed to air or water. Slightly soluble in HCl. Soluble in HNO<sub>3</sub>, H<sub>2</sub>SO<sub>4</sub>. [105],[22],[47]

Form: Bluish-white, lead-like, easily fusible, soft, heavy, malleable metal. It has atomic number 81 (Group IIIA) with valence states of +1 or +3. It does not occur in pure form in nature but is found in the minerals crooksite, lorandite, and hutchinsonite. It leaves a streak on paper and begins to volatilize at 174°C. [108],[51],[22]

Use: Thallium and its compounds are used as rodenticides, fungicides, insecticides, catalysts in certain organic reactions, in phosphor activators, in bromiodide crystals for lenses, plates, and prisms in infrared optical instruments, in photoelectric cells, in mineralogical analysis, alloyed with mercury in low-temperature thermometers, switches and closures, in high-density liquids, in dyes and pigments, and in the manufacture of optical lenses, fireworks, and imitation precious jewelry. The manufacture and distribution of thallium-containing rodenticides and insecticides is no longer permitted. [56]

Fire and explosion hazard: Low.

Flash point: NA

uel: NA

lel: NA

Autoign. temp.: NA

Nonflammable solid. Moderate fire and explosion hazard in the form of dust, when exposed to heat or flame. When heated to decomposition it emits toxic fumes of Tl. Use extinguishing media appropriate to surrounding fire conditions. [51],[55]

Incompatibility: Strong acids; strong oxidizing agents; air sensitive; F<sub>2</sub>. [51],[55]

## 446 - Thallium

**Handling:** WARNING: avoid all contact. Keep away from heat and open flame when in the form of dust. Do not breathe dust or fumes (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (chemical resistant gloves and suit; safety goggles or face shield). Readily absorbed through skin. Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [55],[56]

**Health effects:** Thallium is an extremely toxic and cumulative poison. Routes of entry are inhalation of dust and fumes, ingestion, skin absorption, and eye and skin contact. Points of attack include eye, central nervous system, liver, kidneys, gastrointestinal tract, and body hair. In non-fatal occupational cases of moderate to long-term exposure, early symptoms usually include fatigue, limb pain, metallic taste in the mouth and loss of hair. Later, peripheral neuritis, proteinuria, and joint pains occur. Long-term exposure may produce optic atrophy, paresthesia, and changes in pupillary and superficial tendon reflexes (slowed responses). Acute poisoning rarely occurs and is usually due to ingestion. When it occurs, gastrointestinal symptoms, abdominal colic, loss of kidney function, peripheral neuritis, strabismus, disorientation, convulsions, joint pain, and alopecia develop rapidly (within 3 days). [56],[55]

**Toxicity:** High.

TWA: 0.012 ppm (0.1 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 2.4 ppm (20 mg/m<sup>3</sup>) [56]

Peak: unknown

Odor threshold: unknown

Carcinogenicity: unknown

Mutagenicity: unknown

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: 4.412 mg/kg body wt -- death of an adult male [55]

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown

Toluene

C<sub>7</sub>H<sub>8</sub>

CAS RN: 108-88-3

Syn: Toluene \* Benzene, methyl- \* Antisal 1A \* Methacide \* Methane,  
 phenyl- \* Methylbenzene \* Methylbenzol \* NCI-C07272 \* Phenylmethane \* RCRA  
 Waste Number U220 \* Toluol \* Tolu-sol \* UN 1294 (DOT) \*

Molecular formula: C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub>

Monocyclic Aromatic Hydrocarbon

## Physical properties:

Relative molecular mass:	92.1405	
Specific gravity:	0.867	[104], [107]
	0.86694	[14]
	0.8669	[105], [106]
	0.86683	[49]
	0.8660	[10], [47], [51], [108], [22], [48]
	0.86	[32]
Boiling point:	110.8°C	[47], [104]
	110.7°C	[22], [48]
	110.625°C	[14]
	110.630°C	[49]
	110.6°C	[10], [105], [107], [106], [108]
	110.4°C	[51]
	110.°-111.°C	[56]
	111.°	[32]
Melting point:	-94.5°C	[22]
	-94.991°C	[49]
	-95.° - -94.5°C	[51]
	-95.°C	[10], [105], [107], [32], [106], [108]
	-95.1°C	[104]
Refractive index:	1.4969	[10], [49], [14]
	1.4967	[108]
	1.4961	[105], [107], [106]
	1.497	[22]
Vapor pressure:	0.665 kPa @ -4.4°C (5mm)	[47]
	1.333 @ 6.4°C (10mm)	[104], [105]
	2.667 @ 18.4°C (20mm)	[47]
	2.93 @ 20°C (22mm)	[104], [32]
	3.8036 @ 25°C (28.529mm)	[49]
	4.89 @ 30°C (36.7mm)	[51]
	5.333 @ 31.8°C (40mm)	[104], [105],
Vapor density:	3.14	[104], [32]
Evaporation rate:	1.90	[49], [3]
	2.24	[32]
Relative dielectric permittivity:	2.438 @ 0°C	[105]
	2.44 @ 0°C	[11]
	2.376 @ 20°C (10 kHz)	[2]
	2.385 @ 20°C	[11]
	2.379 @ 25°C	[11], [14]
	2.3807 @ 25°C	[49]
	2.38 @ 25°C	[10]
	2.379 @ 25°C	[105], [20]
	2.364 @ 20°C	[11]
Loss tangent:	unknown	
Relaxation time:	unknown	

# 448 - Toluene

Thermal conductivity:	0.146 W/(m-K) @ -20°C	[20]
	0.1462 @ 0°C	[10]
	0.141 @ 0°C	[20]
	0.1285 @ 12°C	[10]
	0.136 @ 20°C	[20]
	0.1349 @ 20°C	[105]
	0.131 @ 40°C	[20]
	0.126 @ 60°C	[20]
	0.118 @ 80°C	[105]
Electrical resistivity:	$>1 \times 10^6$ MOhm-m	[10]
	$1.25 \times 10^7$	[49]
Critical temperature:	320.8°C	[105]
	318.65°C	[49]
	318.6°C	[107]
	318.57°C	[10]
	320.6°C	[48]
Critical pressure:	4.22 MPa	[105]
	4.109	[10]
	4.108	[107]
	4.106	[49], [20]
Dynamic viscosity:	0.772 mPa-s @ 0°C	[105]
	0.783 @ 0°C	[48]
	0.680 @ 10°C	[48]
	0.590 @ 20°C	[105]
	0.598 @ 20°C	[48]
	0.5525 @ 25°C	[49]
	0.552 @ 25°C	[10]
	0.526 @ 30°C	[105]
	0.4928 @ 35°C	[49]
	0.471 @ 40°C	[105]
	0.354 @ 70°C	[105]
Kinematic viscosity:	0.891 $\mu\text{m}^2/\text{s}$ @ 0°C	
	0.9042 @ 0°C	
	0.7852 @ 10°C	
	0.691 @ 20°C	
	0.681 @ 20°C	
	0.6373 @ 25°C	
	0.637 @ 25°C	
	0.607 @ 30°C	
	0.5685 @ 35°C	
	0.543 @ 40°C	
	0.408 @ 70°C	
Surface tension:	27.7 mN/m @ 10°C vapor	[105]
	28.5 @ 20°C vapor	[105]
	29.0 @ 20°C	[107]
	27.92 @ 25°C	[49]
	27.4 @ 30°C	[20]
	27.33 @ 30°C	[49]
	26.15 @ 40°C	[14]



Contact angle: [18]

	sessile	advancing	receding
quartz	9	10	7
calcite	13	16	5
biotite	12	15	7
Ca-mont.	5	swelled	swelled

Thermal expansion coefficient:	0.001067 K <sup>-1</sup>		[49]
	0.00108		[48]
Compressibility:	0.797 nPa <sup>-1</sup> @ 0°C		[105]
	0.844 @ 10°C		[105]
	0.894 @ 20°C		[105]
	0.91 @ 20°C		[20]
	0.9115 @ 25°C		[49]
	0.949 @ 30°C		[105]
	1.014 @ 40°C		[105]
Vapor diffusivity:	7.6 μm <sup>2</sup> /s @ 0°C		[47]
	8.8 @ 30°C		[47]
Solution diffusivity:	2.09 nm <sup>2</sup> /s in n-decane		[47]
	1.38 in n-dodecane		[47]
	3.72 in n-heptane		[47]
	4.21 in n-hexane		[47]
	1.02 in n-tetradecane		[47]
Electric dipole moment:	1.501x10 <sup>-30</sup> C-m		[10]
	1.20x10 <sup>-30</sup>		[105]
	1.034x10 <sup>-30</sup>		[49]
Ionization potential:	8.82 eV (PI)		[105]
Magnetic volume susceptibility:	-7.765x10 <sup>-6</sup> SI units @ 20°C		[105]
Speed of sound:	1227.2 m/s @ 20.5°C		[15]
Heat of melting:	6.851 kJ/mol		[105]
	6.640		[10]
	6.636		[49]
	6.635		[48]
	6.624		[107], [14]
Heat of vaporization:	39.224 kJ/mol		[105]
	37.991 @ 25°C		[49]
	33.26		[107]
	33.20		[10]
	32.79		[48]
	33.183 @ bp		[49]
	33.48 @ bp		[14]
Heat of sublimation:	38.02 kJ/mol		[10]
Heat capacity @ 25°C:	0.1573 kJ/(mol-K) (liq)		[10]
	0.15729 (liq)		[49]
	0.1561 (liq)		[105]
	0.1038 (gas)		[105]
	0.1037 (gas)		[10]
Heat of combustion:	-3949. kJ/mol @ 20°C (liq)		[105]
	-3736.3 @ 25°C (liq)		[107]
	-3910.07 @ 25°C (liq)		[49]
Heat of formation:	12.02 kJ/mol @ 25°C (liq)		[10]
	11.996 (liq)		[49]
	50.03 (gas)		[10]

## 450 - Toluene

Gibbs (free) energy:	113.8	kJ/mol @ 25°C (liq)	[10]
	122.1		(gas) [10]
Analytical chemistry: $pP_{oct}$ =	2.80		[21]
	2.79		[31]
	2.73		[21], [24], [59]
	2.69 @ 20°C		[104], [8], [21]
	2.65		[12]
	2.21		[4]
	2.11		[21]
	$pK_s$ =	NA	
	$pK_a$ =	>15.	[59]
		NA	[31]
$pK_{BH}$ =	6.3 @ 0°C in HF		[49]
Henry's law constant =	0.601 kPa·m <sup>3</sup> /mol		[24]
	0.68		[41]
	0.683 @ 25°C		[41]
	0.243 dimensionless		[59]
Hydrolysis half-life =	NA		[8]

**Electrochemical data:** Neikam and Desmond (1964), Meites and Zuman (1977), Meites et al. (1977b), Nyberg (1978), Lund (1983a).

**Clay-organic interaction data:** Physical adsorption of toluene and coordination to the exchangeable cations when intercalated by Cu(II) montmorillonite. Frequencies of C-C stretching and C-H out-of-plane vibrations of toluene in the liquid state and when adsorbed by Cu(II) montmorillonite (Pinnavaia and Mortland, 1971; Theng, 1974). Polymerization or oligomerization on interlamellar surfaces of Fe(III) hectorite (Pinnavaia et al., 1974; King and Olhoeft, 1989). Also see [18], Doner and Mortland, 1969; Dragun and Helling, 1985; Rao et al., 1988; Sadowski, 1988.

**Solubility:** Almost insoluble in water. Soluble in acetone. Miscible in ethanol, chloroform, ether, benzene, glacial acetic acid, carbon disulfide. [51], [105], [108], [47], [104], [32], [14]

0.05	wt% in water @ 16°C	[47]
0.0470	wt% in water @ 16°C	[104]
0.05	wt% in water @ 20°C	[32]
0.0515	wt% in water @ 20°C	[104]
7.3	wt% in water @ 25°C	[14]

**Form:** Colorless liquid. Pungent, aromatic, benzene-like odor. Commercial grades may contain up to 5% xylene isomers and small amounts of benzene. [107], [56], [22]

**Use:** In manufacturing benzoic acid, caprolactum, benzaldehyde, toluene diisocyanate, phenol, benzyl and benzoyl derivatives, toluene sulfonates, vinyltoluene, saccharin, explosives (TNT), dyes, and many other organic compounds; as a solvent for paints, lacquers, neoprene, gums, resins, rubber and vinyl organosols; in the extraction of various principles from plants; aviation and high octane blending stock (14.86 wt% [104]); adhesive

solvent in plastic toys and models; dilutor and thinner in nitrocellulose lacquers; detergents; asphalt and naphtha constituent; scintillation counters; 16th highest-volume chemical produced in U.S. (1979). Present in gasoline engine exhaust and vapors. [108],[56],[22],[104]

**Fire and explosion hazard:** Moderate.

Flash point: (CC) 4.4°C [107],[51],[108],[22],[14]

(CC) 4°C [49],[32]

(OC) 12.8°C [107]

uel: 7.0% [107],[51],[22]

7.1% [32]

7.3% [10]

lel: 1.27% [107],[51],[32],[22]

1.0% [10]

Autoign. temp.: 536°C [107],[22]; 480°C [51],[32]

Flammable liquid. Slightly flammable when exposed to heat, flame or oxidizers despite low flash point. Moderately dangerous when heated as it emits irritating fumes (CO and CO<sub>2</sub>). Can react vigorously with oxidizing materials. Fight small fires with CO<sub>2</sub> or dry chemical powder. Use alcohol or polymer foam for large fires. Water may be ineffective. [51],[107]

**Incompatibility:** Strong oxidizers; BrF<sub>3</sub>; 1,3-dichloro-dimethyl-2,4-imidazolidin-2,4-dione; N<sub>2</sub>O<sub>4</sub>; nitric acid; sulfuric acid; tetranitromethane; UF<sub>6</sub>; (H<sub>2</sub>SO<sub>4</sub> + HNO<sub>3</sub>); AgClO<sub>4</sub>. Will attack some forms of plastics, rubber, and coatings. Iron or ferric chloride catalyzes a vigorous exothermic reaction between toluene and sulfur dichloride (Chem. Eng. News, p. 2, August 8, 1988). [32],[56],[55]

**Handling:** Keep away from heat sparks and flame. Avoid breathing vapor or mist (appropriate respirator or self-contained breathing apparatus). Avoid repeated or prolonged skin contact (PVA synthetic latex gloves; lab coat, goggles or face shield). Use with adequate ventilation (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet. Store under nitrogen. Store in secure poison area. [56],[57],[32],[55]

**Health effects:** Toluene is toxic. It is derived from coal tar, and commercial grades usually contain small quantities of benzene as an impurity. Routes of entry are inhalation of vapor, percutaneous absorption of liquid, ingestion, and eye and skin contact. Points of attack include central nervous system, liver, kidneys, and skin. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Inhalation of vapors may cause nausea, vomiting, headache or unconsciousness. Acute poisonings resulting from high concentrations of vapor are rare but can cause lung irritation, chest pain and edema which may be fatal. In the few cases of acute toluene poisoning reported, the effect has been that of a narcotic. Splashed in the eye it may cause irritating but reversible damage. Chronic effects of overexposure may include liver and/or kidney damage, and cardiovascular effects. Toluene is a common air contaminant. [51],[56],[32],[55],[95]

## 452 - Toluene

### Toxicity: Moderate.

TWA: 100 ppm (375 mg/m<sup>3</sup>) [1]

STEL: 150 ppm (560 mg/m<sup>3</sup>) [1]

CL: 200 ppm (750 mg/m<sup>3</sup>) for a 10 min sampling period [51],[56]

IDLH: 2000 ppm (7500 mg/m<sup>3</sup>) [107],[56]

Peak: 500 ppm (1880 mg/m<sup>3</sup>) for 10 min duration [51],[56]

Odor threshold: 0.17-100 ppm (fatigue level at 300-400 ppm) [32]

0.17 ppm (0.62 mg/m<sup>3</sup>) [107]

10-15 ppm (38-56 mg/m<sup>3</sup>) -- detectable by most people [32]

0.6-210 ppm (2.3-790 mg/m<sup>3</sup>) -- detection [104]

3-220 ppm (11-830 mg/m<sup>3</sup>) -- recognition [104]

Carcinogenicity: inconclusive [25]

noncarcinogenic [95]

Mutagenicity: evidence of tetratogenicity [95]

nonmutagenic [95]

inconclusive [37]

### Exposure:

#### External:

Non-lethal: 300 ppm (1130 mg/m<sup>3</sup>) -- eye irritation [51]

Lethal: unknown

#### Oral:

Non-lethal: unknown

Lethal: 0.5 to 5g/kg body wt [107]

50 mg/kg body wt [55]

#### Inhalation:

Short-term Inhalation Limits: 600 ppm (2260 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: 100 ppm (375 mg/m<sup>3</sup>) -- unsatisfactory [104]

200 ppm (750 mg/m<sup>3</sup>) -- CNS effects [51]

200-500 ppm (750-1880 mg/m<sup>3</sup>) -- headache, nausea, eye irritation, loss of appetite, a bad taste, lassitude, impairment of coordination and reaction time [51]

1000 ppm (3750 mg/m<sup>3</sup>)/60 min -- severe toxic effects [104]

Lethal: unknown

## Toxaphene

 $C_{10}H_{10}Cl_8$ 

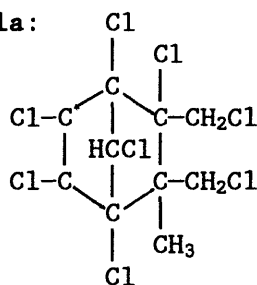
CAS RN: 8001-35-2

Syn: Toxaphene \* Agricide maggot killer (F) \* Alltex \* Alltox \* Anatox \* Attac 4-2 \* Attac 4-4 \* Attac 6 \* Attac 6-3 \* Attac 8 \* Camphechlor \* Camphochlor \* Chem-phene M5055 \* Chlor chem T-590 \* Chlorinated camphene \* Chlorocamphene \* Compound 3956 \* Crestoxo \* Crestoxo 90 \* ENT 9735 \* Estonox \* Fasco-terpene \* Geniphene \* Gy-phene \* Hercules 3956 \* Hercules Motox \* Hercules toxaphene \* Huilex \* Kamfachlor \* M 5055 \* Melipax \* Motox \* NA 2761 \* NCI-C00259 \* Octachlorocamphene \* PCC \* PChK \* Penphene \* Phenacide \* Phenatox \* Phenphane \* Polychlorcamphene \* Polychlorinated camphenes \* Polychlorocamphene \* RCRA Waste Number P123 \* Synthetic 3956 \* Strobane-T \* Strobane-T90 \* Texadust \* Toxakil \* Toxaphen \* Toxon 63 \* Toxyphen \* Vertac 90% \* Vertac toxaphene 90\*

Molecular formula:  $C_{10}H_{10}Cl_8$ 

Polychlorinated Bicyclic Hydrocarbon

Structural formula:



## Physical properties:

Relative molecular mass:	413.813	
Specific gravity:	1.63	[32]
	1.66 @ 27°C	[22]
Boiling point:	decomposes above 120°C	[107], [41]
Melting point:	65.°-90°C	[107], [108], [56], [51], [22]
	70.°-95°C	[32]
Refractive index:	NA	
Vapor pressure:	0.027-0.053 kPa @ 20°C (.2-.4mm)	[32]
Vapor density:	14.3	[32]
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	unknown	
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	

#### 454 - Toxaphene

Speed of sound: unknown  
Heat of melting: unknown  
Heat of vaporization: unknown  
Heat of sublimation: unknown  
Heat capacity @ 25°C: unknown  
Heat of combustion: unknown  
Heat of formation: unknown  
Gibbs (free) energy: unknown

Analytical chemistry:  $pP_{oct}$  - 5.5 [27]  
3.3 [8],[31]  
3.23 - 5.50 [41]  
 $pK_s$  - NA  
 $pK_a$  - NA  
 $pK_{BH}$  - NA  
Henry's law constant - 6.4 kPa-m<sup>3</sup>/mol [41]  
Hydrolysis half-life - 3.15x10<sup>8</sup> sec [8]

Electrochemical data: Unknown

Clay-organic interaction data: LaFleur (1974).

Solubility: Almost insoluble in water. Very soluble in aromatic hydrocarbons and common organic solvents. [51],[22].

0.0003 wt% in water @ 20°C [32]  
0.740 ppm in water @ 25°C [8]  
0.500 ppm in water @ 25°C [8]

Form: Yellow, waxy, solid. Pleasant piney or chlorine-like odor. Toxaphene is a mixture of chlorinated bicyclic terpenes, mainly chlorinated camphene with the approximated formula C<sub>10</sub>H<sub>10</sub>Cl<sub>8</sub>. Contains 67-69% chlorine. Solid sinks in water, solution floats on water. Dehydrochlorinates in the presence of alkali, prolonged exposure to sunlight, and at temperatures of about 155°C. [22],[104],[51],[107],[108],[41]

Use: The largest simple use is as pesticide on cotton crops. Other major uses are on cattle and swine, and on soybeans, corn, wheat, and peanuts. Substantial amounts also are used for lettuce, tomatoes, and other food crops. [104]

Fire and explosion hazard: Low.

Flash point: (CC) 135°C [32]  
(CC) 29.9°C (solution) [107]

uel: 6.4% [107]

lel: 1.1% [107]

Autoign. temp.: 530°C (solution) [107]

Flammable liquid; nonflammable solid. When heated to decomposition, it emits toxic fumes of chlorine gas. Fight fire with dry chemical powder, CO<sub>2</sub>. [107],[32],[51]

Incompatibility: Strong oxidizing agents. [32]

**Handling:** WARNING: avoid all contact. Prevent inhalation of vapor, dust or mist (appropriate respirator or self-contained breathing apparatus). Wear appropriate clothing and eye protection to prevent any possibility of skin and eye contact with liquid toxaphene or repeated or prolonged skin contact with solid toxaphene. Wash immediately if skin is wet or contaminated with liquid toxaphene, promptly when contaminated with solid toxaphene. Work clothing should be changed daily if it is possible that clothing is contaminated with solid toxaphene. Remove clothing immediately if wet with liquid toxaphene and promptly remove if contaminated with solid toxaphene. Provide emergency showers. Keep container tightly closed. Store in cool, dry, secure poison area. [56]

**Health effects:** Toxaphene is a poison and possible carcinogen. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin. Points of attack include skin and central nervous system. Overexposure can cause central nervous system stimulation. Overexposure may also cause nausea, mental confusion, agitation, involuntary trembling, convulsions, unconsciousness, and possible death. Contact may cause irritation of the skin. A single dermal application of 46 grams or daily application of 2.4 grams is dangerous. [32],[51],[108]

**Toxicity:** Very high.

TWA: 0.030 ppm (0.5 mg/m<sup>3</sup>) [1]

STEL: 0.059 ppm (1 mg/m<sup>3</sup>) [1]

CL: unknown

IDLH: 11.8 ppm (200 mg/m<sup>3</sup>) [107],[56]

Peak: unknown

Odor threshold: 0.14 mg/kg in water [104]

Carcinogenicity: possible human carcinogen [51]  
animal positive [51]

Mutagenicity: unknown

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: 40 mg/kg body wt [51]

2-7 g [32]

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: unknown

Lethal: unknown

## 456 - 1,2,4-Trichlorobenzene

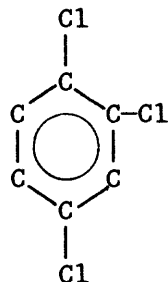
1,2,4-Trichlorobenzene

 $C_6H_3Cl_3$ 

CAS RN: 120-82-1

Syn: 1,2,4-Trichlorobenzene \* Benzene, 1,2,4-trichloro- \* Hostetex L-PEC \*  
 1,2,4-TCB \* unsym-Trichlorobenzene \* 1,2,5-Trichlorobenzene \* 1,3,4-  
 Trichlorobenzene \* 1,2,4-Trichlorobenzol \* UN 2321 (DOT) \*

Structural formula:



Polychlorinated Aromatic Hydrocarbon

## Physical properties:

Relative molecular mass:	181.449	
Specific gravity:	1.446 @ 25°C	[10]
	1.454 @ 25/25	[51]
	1.4542	[14], [105]
	1.4634 @ 25°C	[22]
	1.4634 @ 25/25	[108]
Boiling point:	213.°C	[108], [104], [51], [22]
	213.48°C	[14]
	213.5°C	[56], [105]
	214.°C	[10]
Melting point:	16.95°C	[14]
	17.°C	[108], [105], [104], [51], [22], [10]
Refractive index:	1.5717	[14], [105]
	1.5707 @ 20°C	[10]
	1.5524 @ 25°C	[108]
Vapor pressure:	0.0388 kPa @ 25°C (0.2907mm)	[14], [23]
	0.133 @ 38.4°C (1mm)	[105], [51], [47]
	1.33 @ 81.7°C (10mm)	[105]
Vapor density:	6.25	[104]
	6.26	[51]
Evaporation rate:	unknown	
Relative dielectric permittivity:	6.75 @ 20°C (1.8 MHz)	[2]
	3.945 @ 25°C	[14]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	1.4225 mPa·s @ 20°C	[14]
	1.0252 @ 40°C	[14]
Kinematic viscosity:	0.9782 $\mu m^2/s$ @ 20°C	
	0.7050 @ 40°C	
Surface tension:	39.10 mN/m @ 20°C	[14]
	37.98 @ 30°C	[14]
	36.86 @ 40°C	[14]



Contact angle: [18]

	sessile	advancing	receding
quartz	28	28	17
calcite	36	33	16
biotite	28	27	8
Ca-mont.	6	9	5

Thermal expansion coefficient: unknown

Compressibility: unknown

Vapor diffusivity: unknown

Solution diffusivity: unknown

Electric dipole moment: unknown

Ionization potential: unknown

Magnetic volume susceptibility: unknown

Speed of sound: unknown

Heat of melting: 16.36 kJ/mol [14]

Heat of vaporization: 47.83 kJ/mol [105]

43.63 [14]

Heat of sublimation: unknown

Heat capacity @ 25°C: 0.1946 kJ/(mol-K) [105]

Heat of combustion: unknown

Heat of formation: unknown

Gibbs (free) energy: unknown

Analytical chemistry:  $pP_{oct}$  = 4.28 [31]

4.26 [8]

4.04 [27]

4.02 [23]

3.98 [12]

$pK_s$  = NA

$pK_a$  = NA [31]

$pK_{BH}$  = NA

Henry's law constant = 0.235 kPa-m<sup>3</sup>/mol [41]

0.12 [96]

Hydrolysis half-life = NA [8]

Electrochemical data: Unknown

Clay-organic interaction data: Chiou et al. (1983)

Solubility: Almost insoluble in water. Slightly soluble in ethanol.

Miscible with ether, benzene, carbon disulfide, and most organic solvents and oils. [108],[22],[10],[104]

19. ppm in water at 22°C [104]

0.0049 wt% in water @ 20°C [23]

0.0031 wt% in water @ 25°C [41]

Form: Colorless crystals, clear stable liquid. Aromatic odor similar to o-dichlorobenzene. [104],[51],[41]

Use: Solvent in chemical manufacturing; dyes and intermediates; dielectric fluid in transformers; synthetic transformer oils; lubricants; heat-transfer medium; degreaser; potential insecticide against termites. 46% of use is as a dye carrier; 28% as a herbicide intermediate. [104],[22],[56]

## 458 - 1,2,4-Trichlorobenzene

**Fire and explosion hazard:** Low.

Flash point: (OC) 98.9°C [22]  
(CC) 110°C [51],[108],[14]

uel: 6.6 @ 150°C [55]

lel: 2.5% [55]

Autoign. temp.: unknown

Slightly flammable liquid. Low fire hazard when exposed to heat or flame. Emits toxic fumes of CO, CO<sub>2</sub>, and hydrogen chloride gas when heated to decomposition. Fight fire with water spray, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [51],[55]

**Incompatibility:** Can react vigorously with oxidizing materials. [51]

**Handling:** Avoid heat and flame. Do not breathe vapor or mist (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, on clothing (chemical resistant gloves; safety goggles; other protective clothing). Use with adequate ventilation (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area. [57],[55]

**Health effects:** 1,2,4-Trichlorobenzene is an irritant. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include skin, eyes, liver, kidneys, and lungs. Vapor or mist is irritating to the skin, eyes, mucous membranes and upper respiratory tract. Prolonged or repeated contact with liquid may cause skin burns. Acute exposure may cause drowsiness, incoordination, and unconsciousness. Chronic effects include nausea, dizziness and headache, gastrointestinal disturbances, damage to the liver, kidney and lung. [56],[55]

**Toxicity:** Unknown

TWA: no value set [1]

STEL: no value set [1]

CL: 5 ppm (40 mg/m<sup>3</sup>) [1]

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: unknown

Mutagenicity: unknown

**Exposure:** Unknown

1,1,1-Trichloroethane

 $C_2H_3Cl_3$ 

CAS RN: 71-55-6

Syn: 1,1,1-Trichloroethane \* Ethane, 1,1,1-trichloro- \* Aerothane \*  
 Aerothene \* Aerothene TT \* Baltana \* Chloroetene \* Chloroethene \*  
 Chlorotene \* Chlorothane NU \* Chlorothene \* Chlorothene NU \* Chlorothene VG  
 \* Chlorten \* Genklene \* Inhibisol \* Methylchloroform \* Methyl chloroform \*  
 Methyltrichloromethane \* NCI-C04626 \* RCRA Waste Number U226 \* Solvent III  
 \* Strobane \*  $\alpha$ -T \* 1,1,1-TCA \* 1,1,1-TCE \* Trichloroethane \*  $\alpha$ -  
 Trichloroethane \* Tri-ethane \* UN 2831 (DOT) \*

Molecular formula:  $H_3C-CCl_3$ 

Polychlorinated Aliphatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	133.4047	
Specific gravity:	1.3390	[105], [16]
	1.3381	[49]
	1.3376	[10], [51], [108]
	1.35	[104]
	1.33	[32]
Boiling point:	1.31	[107]
	81.°C	[104]
	75.°C	[22]
	74.083°C	[49]
	74.°C	[10], [32], [107], [56]
	74.1°C	[105], [51], [47], [108], [16]
Melting point:	71.°C	[104]
	-30.4°C	[10], [49], [105]
	-32.°C	[104]
	-32.5°C	[51], [108]
	-32.7°C	[10]
	-38.°C	[32], [22]
Refractive index:	<-39.°C	[107]
	1.43838	[108]
	1.4380	[49]
	1.4379	[10], [105], [16]
Vapor pressure:	4.9 kPa @ 0°C (37mm)	[41]
	5.333 @ 1.6°C (40mm)	[105], [47]
	8.00 @ 9.5°C (60mm)	[47]
	8.3 @ 10°C (62mm)	[41]
	13.33 @ 20°C (100mm)	[104], [105], [51]
	16.49 @ 25°C (113.7mm)	[49]
	20.66 @ 30°C (155mm)	[104]
	32.0 @ 40°C (240mm)	[41]
	45.3 @ 50°C (340mm)	[41]
Vapor density:	4.55	[32]
	4.63	[104]
	4.6	[107]
Evaporation rate:	12.8	[32]
	6.0	[49]
Relative dielectric permittivity:	7.953 @ 0°C	[49], [10]
	7.1 @ 7°C	[11]
	7.252 @ 19.8°C	[49]
	7.52 @ 20°C	[11]
	7.68 @ 20°C	[10]

# 460 - 1,1,1-Trichloroethane

Loss tangent:	unknown	
Relaxation constant:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	1.37 MOhm-m	[49]
Critical temperature:	272.°C	[49]
Critical pressure:	4.3	[49]
Dynamic viscosity:	0.903 mPa-s @ 15°C	[10]
	1.2 @ 20°C	[105]
	0.795 @ 25°C	[49]
	0.725 @ 30°C	[49]
Kinematic viscosity:	0.674 μm <sup>2</sup> /s @ 15°C	
	0.897 @ 20°C	
	0.594 @ 25°C	
	0.541 @ 30°C	
Surface tension:	26.17 mN/m @ 15°C	[49]
	25.56 @ 20°C	[49]
	25.4 @ 20°C	[107], [16]
	25.39 @ 20°C	[15]
	24.25 @ 30°C	[49]
	24.24 @ 30°C	[16]
	24.11 @ 30°C	[15]
	23.09 @ 40°C	[16]
	22.87 @ 40°C	[15]
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	7.9 μm <sup>2</sup> /s @ 25°C	[59]
Solution diffusivity:	0.8 nm <sup>2</sup> /s (calc)	[59]
Electric dipole moment:	5.971x10 <sup>-30</sup> C-m	[10]
	5.67x10 <sup>-30</sup>	[49]
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	2.350 kJ/mol	[49]
	2.734	[105]
	1.884	[10]
Heat of vaporization:	29.708 kJ/mol	[49]
	32.0184	[107]
	33.547	[105]
	33.327	[10]
Heat of sublimation:	32.500 kJ/mol	[10]
Heat capacity @ 25°C:	0.1444 kJ/(mol-K) (liq)	[49]
	0.1439 (liq)	[105]
	0.0937 (gas)	[105]
	0.09240 (gas)	[10]
Heat of combustion:	-1108.05 kJ/mol @ 25°C (liq)	[49]
Heat of formation:	-178.82 kJ/mol @ 25°C (liq)	[49]
	-142.3 (gas)	[49]
	-142.39 (gas)	[10]
Gibbs (free) energy:	-76.24 kJ/mol @ 25oC (gas)	[10]

Analytical chemistry:	pPoc <sub>t</sub> =	2.50	[31]
		2.49	[21],[24],[59]
		2.47	[4],[27]
		2.17	[8]
	pK <sub>s</sub> =	NA	
	pK <sub>a</sub> =	NA	[31]
	pK <sub>BH</sub> =	NA	
Henry's law constant =		0.8 kPa·m <sup>3</sup> /mol	[24]
		1.32 - 2.78	[41]
		0.201 dimensionless	[59]
Hydrolysis half-life =		1.6x10 <sup>7</sup> sec	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Karickhoff (1981).

Solubility: Almost insoluble in water. Soluble in acetone, benzene, carbon tetrachloride, methanol. Miscible with ethanol and ether. Absorbs some water. [10],[51],[108],[32],[49],[104]

0.07	wt% water @ 20°C	[32]
0.132	wt% water @ 20°C	[10],[49]
0.44	wt% water @ 20°C	[104]
0.1495	wt% water @ 25°C	[96]

Form: Colorless liquid. Mild, sweetish odor like chloroform. Ketones, alcohols, esters, or nitrogen compounds may be added as stabilizers or inhibitors. Some commercial grades may be inhibited with 3% 1,4-dioxane. [55],[51],[32],[22]

Use: Solvent in cold cleaning of metals and plastics; vapor degreasing; ultrasonic cleaning; dyeing and cleaning of yarns; polymer manufacture; primary and carrier solvent in spot cleaners, adhesives, shoe polishes, stain repellents, hair sprays, Mace, insecticides, resins, inks, lubricants, protective coatings, asphalt extraction, and waste water treatment; during printed circuit board production; liquid Drano production; photographic film processing; propellant. [56],[22],[108]

Fire and explosion hazard: Very low.

Flash point: none with normal testing methods [32],[49],[22]

uel: 16% [32],[107]

12.5% [41]

lel: 7% [32],[107]

7.5% [41]

Autoign. temp.: 500°C [32],[107]

Nonflammable liquid but dangerous. May decompose to form toxic and irritant fumes of hydrogen chloride, chlorine, phosgene, hydrochloric acid, dichloroacetylene, and carbon monoxide upon contact with hot metal or exposure to ultraviolet radiation. Reacts slowly with water to form hydrochloric acid. Contact with strong caustics, strong oxidizers, and chemically active metals may cause fire or explosion. Fight fire with water spray, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam.

[51],[56],[107],[32],[108],[55]

## 462 - 1,1,1-Trichloroethane

**Incompatibility:** Water; strong bases; chemically active metals such as aluminum and its alloys, magnesium powders, sodium, potassium, zinc; strong oxidizing agents. Reacts violently with  $\text{N}_2\text{O}_4$ ,  $\text{O}_2$ ,  $\text{O}_2$  liquid, Na, NaOH, Na-K alloy. 1,1,1-trichloroethane has been reported to react violently with acetone, nitrites, and oxygen. [56],[32],[55]

**Handling:** WARNING: 1,4-dioxane is a cancer-suspect agent. Avoid moisture, insufficient inhibitor, heat, flame, other sources of ignition, sunlight and ultraviolet light. Prevent inhalation vapor or mist (appropriate respirator or self-contained breathing apparatus). Prevent repeated or prolonged eye or skin contact (leather, neoprene or polyvinyl alcohol gloves; lab coat and boots, chemical safety goggles and face shield). It attacks natural rubber. Readily corrodes aluminum and its alloys. Safety shower and eye bath should be available. Use with adequate ventilation (fume hood). Keep container tightly closed. Handle and store under nitrogen. Suitable for general chemical storage in a cool, dry place. Store in secure poison area. [32],[57],[107],[56],[55],[41]

**Health effects:** 1,1,1-Trichloroethane is an irritant and has narcotic properties. Routes of entry are inhalation of vapor, moderate skin absorption, ingestion, and eye and skin contact. Points of attack include skin, eyes, mucous membranes and upper respiratory tract, liver, kidneys, cardiovascular system, gastrointestinal system, and central nervous system. Short-term exposure to vapor may cause headache, dizziness, drowsiness, unconsciousness, irregular heart beat and death. It may cause irritation if splashed in the eyes. Prolonged or repeated skin contact may cause irritation, and dry, scaly and fissured dermatitis. Chronic effects of overexposure may include liver and/or kidney damage. It is narcotic in high concentrations. Causes a proarrhythmic activity which sensitizes the heart to epinephrine induced arrhythmias. This sometimes may cause a cardiac arrest if massively inhaled. [32],[51],[56],[55],[96]

**Toxicity:** Moderate.

TWA: 350 ppm (1900 mg/m<sup>3</sup>) [1]

STEL: 450 ppm (2450 mg/m<sup>3</sup>) [1]

CL: 350 ppm (1910 mg/m<sup>3</sup>) within any 15 min period [51]

IDLH: 1000 ppm (5460 mg/m<sup>3</sup>) [107],[56]

Peak: 800 ppm (4360 mg/m<sup>3</sup>) for 5 min in a 2 hr period [51]

Odor threshold: 100 ppm (545 mg/m<sup>3</sup>) [107]

2000 ppm (10,900 mg/m<sup>3</sup>) -- detection [104]

700-3000 ppm (3800-16,400 mg/m<sup>3</sup>) -- recognition [104]

20-400 ppm (110-220 mg/m<sup>3</sup>) [32]

Carcinogenicity: indefinite [51]

negative in small animals [40]

Mutagenicity: indefinite [96]

nonmutagenic [30]

**Exposure:**

**External:**

Non-lethal: 450 ppm (2450 mg/m<sup>3</sup>) for 8 hr -- eye irritation [51]  
500 ppm for 180 min -- eye irritation, headache [104],[32]

Lethal: unknown

**Oral:**

Non-lethal: 670 mg/kg body wt -- gastrointestinal tract effects [51]

Lethal: unknown

**Inhalation:**

Short-term Inhalation Limits: 1000 ppm (5460 mg/m<sup>3</sup>) for 60 min [107]

Non-lethal: 920 ppm (5020 mg/m<sup>3</sup>) for 70 min -- CNS effects [51]

350 ppm (1900 mg/m<sup>3</sup>) -- psychotropic effects [51]

1000 ppm for 15 min -- disturbance of equilibrium [32]

>1700 ppm -- minor disturbance of equilibrium, headache [32]

2000 ppm for 5 min -- disturbance of equilibrium [32]

5000 ppm/5 min -- marked incoordination, anesthesia [32]

Lethal: 5000 ppm (27 g/m<sup>3</sup>) for 10 min [51]

## 464 - 1,1,2-Trichloroethane

1,1,2-Trichloroethane

 $C_2H_3Cl_3$ 

CAS RN: 79-00-5

Syn: 1,1,2-Trichloroethane \* Ethane, 1,1,2-trichloro- \* Ethane trichloride  
 \* NCI-C04579 \* RCRA Waste Number U227 \* RCRA Waste Number U359 \*  $\beta$ -T \*  
 beta-T \* 1,1,2-TCA \* 1,1,2-Trichlorethane \*  $\beta$ -Trichloroethane \* beta-  
 Trichloroethane \* 1,2,2-Trichloroethane \* Vinyl trichloride \*

Molecular formula:  $ClCH_2-CHCl_2$ 

Polychlorinated Aliphatic Hydrocarbon

## Physical properties:

Relative molecular mass:	133.405	
Specific gravity:	1.4432	[22]
	1.4416	[10], [51], [108]
	1.44	[104]
	1.4397	[105], [16]
	1.43931	[49]
	1.43	[32]
Boiling point:	114.°C	[51]
	113.85°C	[49]
	113.8°C	[105]
	113.7°C	[104], [22], [16]
	113.5°C	[10]
	113.°C	[32], [56]
	113.°-114°C	[108]
Melting point:	-35.°C	[104], [51], [108]
	-36.4°C	[22]
	-36.5°C	[105]
	-36.53°C	[49]
	-36.7°C	[104], [10]
	-37.°C	[32]
Refractive index:	1.4706	[10]
	1.4711	[108]
	1.47124	[49]
	1.4714	[105], [16]
Vapor pressure:	0.667 kPa @ -2.0°C (5mm)	[47]
	1.333 @ 8.3°C (10mm)	[105], [47]
	2.23 @ 20°C (24mm)	[22]
	2.506 @ 20°C (18.8mm)	[32]
	2.533 @ 20°C (19mm)	[104]
	2.667 @ 21.6°C (20mm)	[47]
	2.998 @ 25°C (22.49mm)	[49]
	4.266 @ 30°C (32mm)	[104]
	5.333 @ 35°C (40mm)	[104]
	5.333 @ 35.2°C (40mm)	[51], [47]
Vapor density:	4.63	[104]
	4.55	[32]
Evaporation rate:	1.9	[49]
Relative dielectric permittivity:	8.78 @ 20°C	[10]
	7.288 @ 20°C	[2]
	7.29 @ 20°C	[49]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	



Critical temperature:	339.°C	[49]
Critical pressure:	4.834 MPa	[49]
Dynamic viscosity:	0.119 mPa-s @ 20°C	[10]
Kinematic viscosity:	0.0825 $\mu\text{m}^2/\text{s}$ @ 20°C	
Surface tension:	34.01 mN/m @ 20°C	[16]
	33.75 @ 20°C	[49]
	33.00 @ 25°C	[49]
	22.0 @ 25°C	[105]
	32.55 @ 30°C	[16]
Contact angle:	unknown	
Thermal expansion coefficient:	0.00100 K <sup>-1</sup> @ 0°-25°C	[49]
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	4.7x10 <sup>-30</sup> C-m (gas)	[49]
	5.27x10 <sup>-30</sup>	[105]
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	11.543 kJ/mol	[49], [105]
	11.30	[10]
Heat of vaporization:	38.365 kJ/mol	[105]
	34.75	[10]
	34.23	[49]
Heat of sublimation:	39.36 kJ/mol	[10]
Heat capacity @ 25°C:	0.0899 kJ/(mol-K) (gas)	[10]
@ 20°C:	0.1485 (liq)	[49]
Heat of combustion:	-1098.1 kJ/mol (liq)	[46]
Heat of formation:	-188.5 kJ/mol @ ?? (liq)	[46]
	-182.0 @ 25°C (liq)	[49]
	-148.2 @ ?? (gas)	[46]
	-142.01 @ 25°C (gas)	[49]
	-138.58 (gas)	[10]
Gibbs (free) energy:	-77.54 kJ/mol @ 25°C (gas)	[10]
Analytical chemistry: p <sub>Oct</sub> =	2.42	[27]
	2.38	[97]
	2.18	[41]
	2.17	[8]
	2.07	[31]
	2.07 (calc)	[24]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	0.075 kPa-m <sup>3</sup> /mol	[41]
	0.12 @ 20°C	[24]
	0.0921 @ 25°C	[41]
	0.150 @ 37°C	[41]
Hydrolysis half-life =	1.6x10 <sup>7</sup> sec (est)	[8]

Electrochemical data: Unknown

Clay-organic interaction data: Unknown

## 466 - 1,1,2-Trichloroethane

**Solubility:** Almost insoluble in water. Soluble in chloroform. Miscible with ethanol, ether. [108],[10],[32],[49],[104]

0.44 vol% in water @ 20°C [49]

0.45 wt% in water @ 20°C [32],[104]

0.48 wt% in water @ 25°C [10]

**Form:** Colorless liquid. Pleasant sweet odor, like chloroform. [51],[108]

**Use:** Chemical intermediate in manufacture of 1,1-dichloroethylene; solvent for chlorinated rubber and various organic materials such as fats, oils, resins, waxes, etc.; fumigant; organic synthesis. [108],[56],[41]

**Fire and explosion hazard:** Very low.

Flash point: NA

UEL: 15.5% (high energy ignition source required) [32]

LEL: 6.0% (high energy ignition source required) [32]

Autoign. temp.: NA

Nonflammable liquid. May emit hazardous CO, CO<sub>2</sub>, hydrogen chloride gas, and phosgene gas when heated to decomposition. [108],[51],[55]

**Incompatibility:** Strong oxidizers; strong caustics; chemically active metals such as aluminum, magnesium powders, sodium, potassium. Attacks natural rubber. [56],[51],[55]

**Handling:** Avoid heat. Do not breathe vapor (appropriate respirator or self-contained breathing apparatus). Avoid prolonged or repeated exposure. Do not get in eyes, on skin, on clothing (leather, polyvinyl alcohol, or neoprene gloves and overclothing; safety goggles). Attacks natural rubber. Wash promptly when skin is wet or contaminated. Remove nonimpervious clothing promptly if wet or contaminated. Keep container tightly closed. Store in a cool, dry, secure poison area. [56],[55]

**Health effects:** 1,1,2-Trichloroethane is an irritant and has narcotic properties. Routes of entry are inhalation, skin absorption, ingestion, and eye and skin contact. Points of attack include central nervous system, eyes, respiratory system, liver, and kidneys. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Short-term exposure may cause drowsiness, incoordination, unconsciousness, and death. Chronic exposure might cause liver or kidney damage. Exposure to and/or consumption of alcohol may increase toxic effects. [32],[56],[55],[97]

**Toxicity:** Moderate

TWA: 10 ppm (45 mg/m<sup>3</sup>) (skin) [1]

STEL: no value set [1]

CL: unknown

IDLH: 500 ppm (2730 mg/m<sup>3</sup>) [56]

Peak: unknown

Odor threshold: unknown

Carcinogenicity: suspected animal [51],[104]

possible human [55]

indefinite [40]

Mutagenicity: inconclusive [97]

**Exposure:** Unknown

Trichloroethene

 $C_2HCl_3$ 

CAS RN: 79-01-6

Syn: Trichloroethene \* Ethene, trichloro- \* Acetylene trichloride \*  
 Algylen \* Anamenth \* Benzinol \* Blacosolv \* Blancosolv \* Cecolene \*  
 Chorilen \* 1-Chloro-2,2-dichloroethylene \* Chlorylea \* Chlorylen \* Chorylen  
 \* Circosolv \* Crawhaspol \* Densinfluat \* 1,1-Dichloro-2-chloroethylene \*  
 Dow-Tri \* Dukeron \* Ethinyl trichloride \* Ethylene trichloride \* Ethylene,  
 trichloro- \* Flek-flip \* Flock-flip \* Fluate \* Gemalgene \* Germalene \*  
 Germalgene \* Lanadin \* Lethurin \* Narcogen \* Narkogen \* Narkosoid \* NCI-  
 C04546 \* Nialk \* Perm-a-chlor \* Perm-a-clor \* Petzinol \* Philex \* RCRA  
 Waste Number U228 \* TCE \* Threthylen \* Threthylene \* Trethylene \* Tri \*  
 Triad \* Trial \* Triasol \* Trichloran \* Trichloren \* Trichloroethylene \*  
 1,1,2-Trichloroethylene \* 1,2,2-Trichloroethylene \* 1,1,2-Trichloroethene \*  
 1,2,2-Trichloroethene \* Tri-clene \* Triclören \* Trielene \* Trielin \*  
 Triklone \* Trilen \* Trilene \* Triline \* Trimar \* Triol \* Tri-plus \* Tri-  
 plus M \* UN 1710 (DOT) \* Vestrol \* Vextrol \* Vitran \* Westrosol \*

Molecular formula:  $ClCH=CCl_2$ 

Polychlorinated Aliphatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	131.3889		
Specific gravity:	1.4649		[10], [51]
	1.4642		[105], [15]
	1.464		[48]
	1.46		[104], [107]
	1.4694		[108]
Boiling point:	87.19°C		[49]
	87.°C		[105], [107]
	86.8°C		[48]
	86.7°C	[10], [104], [51], [22],	[108]
	86.°-87°C		[56]
Melting point:	-84.8°C		[10], [108]
	-86.4°C		[107], [49], [48]
	-86.8°C		[51]
	-87.°C		[104]
Refractive index:	1.45560 @ 25°C		[108]
	1.4773		[105]
	1.4775		[10]
	1.47914 @ 17°C		[108]
Vapor pressure:	1.333 kPa @ -12.4°C	(10mm)	[105], [47]
	2.666 @ -1°C	(20mm)	[47]
	2.666 @ 0°C	(20mm)	[104]
	5.333 @ 11.9°C	(40mm)	[105], [47]
	6.307 @ 25°C	(47.3mm)	[49]
	7.73 @ 20°C	(58mm)	[3]
	8.00 @ 20°C	(60mm)	[104], [47]
	12.666 @ 30°C	(95mm)	[104]
	13.332 @ 31.4°C	(100mm)	[105], [47]
	13.332 @ 32°C	(100mm)	[51]
Vapor density:	4.54		[104]
	4.53		[105], [51], [108]
	4.5		[107]
Evaporation rate:	4.46		[49]

# 468 - Trichloroethene

Relative dielectric permittivity:	3.42 @ 10°C	[11]
	3.42 @ 16°C	[49], [10], [105]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.116 W/(m-K) @ 20°C	[105]
	0.138 @ 50°C	[48]
Electrical resistivity:	1.25 MOhm-m @ 20°C	[49]
Critical temperature:	298.°C	[49], [3]
	271.°C	[10]
Critical pressure:	4.91 MPa	[49], [3]
	5.02	[10]
Dynamic viscosity:	0.71 mPa-s @ 0°C	[48]
	0.64 @ 10°C	[48]
	0.58 @ 20°C	[48]
	0.566 @ 20°C	[10], [49]
	0.532 @ 25°C	[49]
	0.53 @ 30°C	[48]
	0.517 @ 30°C	[49]
Kinematic viscosity:	0.486 $\mu\text{m}^2/\text{s}$ @ 0°C	
	0.438 @ 10°C	
	0.397 @ 20°C	
	0.387 @ 20°C	
	0.363 @ 25°C	
	0.363 @ 30°C	
	0.353 @ 30°C	
Surface tension:	29.5 mN/m @ 20°C	[49]
	29.28 @ 20°C	[15]
	29.3 @ 20°C	[107]
	28.8 @ 25°C	[49]
	27.94 @ 30°C	[15]
	26.76 @ 40°C	[15]
Contact angle:	unknown	
Thermal expansion coefficient:	0.00117 K <sup>-1</sup>	[49]
	0.00119	[48]
Compressibility:	0.857 nPa <sup>-1</sup> @ 25°C	[105]
Vapor diffusivity:	8.8 $\mu\text{m}^2/\text{s}$ @ 25°C	[59]
Solution diffusivity:	0.83 nm <sup>2</sup> /s	[59]
Electric dipole moment:	3.002x10 <sup>-30</sup> C-m	[10]
	2.669x10 <sup>-30</sup> in CCl <sub>4</sub>	[49]
Ionization potential:	9.45 eV (PI)	[105]
Magnetic volume susceptibility:	-9.22x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	31.0 kJ/mol	[15]
	31.4	[48]
	31.5	[107], [10]
	31.47 @ bp	[49]
	34.27 @ 25°C	[49]
	34.812	[105]
Heat of sublimation:	34.3 kJ/mol	[10]

Heat capacity @ 25°C:	0.1206 kJ/(mol-K)	(liq)	[105]
	0.1218	(liq)	[108]
	0.1226	(liq)	[49]
	0.0794	(gas)	[108]
	0.0803	(gas)	[10], [105]
Heat of combustion:	-962.37 kJ/mol @ 18°C	(liq)	[49]
Heat of formation:	-42.3 kJ/mol @ 25°C	(liq)	[49], [105]
	-7.78	(gas)	[49], [105]
	-5.862	(gas)	[10]
Gibbs (free) energy:	12.14 kJ/mol @ 25°C	(liq)	[105]
	19.89	(gas)	[10]
	18.04	(gas)	[105]
Analytical chemistry: $pP_{oct}$ =	2.53		[27]
	2.42		[4], [31], [24], [59]
	2.29		[50], [8], [21]
	2.29 - 3.30		[41]
$pK_s$ =	NA		
$pK_a$ =	NA		[31]
$pK_{BH}$ =	NA		
Henry's law constant =	1.04 kPa-m <sup>3</sup> /mol		[24]
	1.19		[41]
	0.92		[41]
	1.0 @ 20°C		[41]
	2.00 @ 37°C		[41]
	0.3729 dimensionless (calc)		[59]
Hydrolysis half-life =	2.8x10 <sup>7</sup> sec		[8]

**Electrochemical data:** Unknown

**Clay-organic interaction data:** Trichloroethene increases the hydraulic conductivity of clay soils (Brown and Thomas, 1984; Anderson et al., 1985). Sorption of trichloroethene on soil and clay (Rogers and McFarlane, 1981; Rao et al., 1988).

**Solubility:** Slightly soluble in water. Soluble in acetone. Miscible with ethanol, ether, chloroform. Dissolves most fixed and volatile oils. [10], [104], [47], [49]

0.11 wt% in water @ 20°C	[8]
0.11 wt% in water @ 25°C	[10], [47], [104]
0.137 wt% in water @ 25°C	[49]

**Form:** Clear, colorless liquid. Characteristic sweet, chloroform-like or ether-like odor. [51], [22], [56], [104]

**Use:** In very large quantities as a metal degreaser and dry cleaning agent (>90% of produced TCE); solvent for fats, waxes, resins, oils, rubbers, paints, varnishes, cellulose esters and ether; manufacture of organic chemicals, pharmaceuticals such as chloroacetic acid; textiles; refrigerant and heat exchange liquid; fumigant; aerospace operations (flushing liquid oxygen); extraction of caffeine from coffee. [56], [22]

#### 470 - Trichloroethene

**Fire and explosion hazard:** Very low.

Flash point: (CC) 32.2°C [107]

(CC) 32°C [51]

uel: 90% above 30°C [51]

10.5% [107]

lel: 12.5% @ 57°C [55]

8.0% [107]

Autoign. temp.: 420°C [51]

410°C [107]

Practically nonflammable liquid at normal temperatures but dangerous. High concentrations of TCE vapor in high-temperature air can be made to burn mildly if plied with a strong flame. Can be dangerous when heated to decomposition as it emits toxic fumes of CO, CO<sub>2</sub>, chlorine gas, phosgene and hydrogen chloride. Liquid or vapor in contact with flames or hot glowing surfaces may form corrosive acids. Fight fire with dry chemical powder, CO<sub>2</sub>, alcohol or polymer foam, water fog. [51],[107]

**Incompatibility:** Can react violently with aluminum, barium, beryllium, lithium, magnesium, sodium, N<sub>2</sub>O<sub>4</sub>, liquid O<sub>2</sub>, O<sub>3</sub>, KOH, KNO<sub>3</sub>, NaOH, titanium; oxidizing agents; reducing agents; strong bases; light. Reaction with alkali may form dichloroacetylene. [51],[56],[104],[55]

**Handling:** Keep away from heat, light, sources of ignition, and flame. Prevent inhalation of vapor or mist (appropriate respirator or self-contained breathing apparatus). Prevent all contact with skin, eyes, and clothing (PVA synthetic latex gloves; lab coat, chemical safety goggles, face shield). Use with adequate ventilation (fume hood). Safety shower and eye bath should be provided. Keep container tightly closed. Preserve in sealed, light-resistant ampoules or in non-breakable, light-resistant glass tubes. Keep container tightly closed. Store in cool, dry, secure poison area or cabinet. [107],[56],[57],[55]

**Health effects:** Trichloroethene is a strong irritant and human carcinogen. Routes of entry are inhalation, percutaneous absorption, ingestion, and eye and skin contact. Points of attack include respiratory system, cardiovascular system, liver, kidneys, central nervous system, gastrointestinal system, and skin. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. Moderate exposures can cause symptoms similar to alcohol inebriation. Higher concentrations can have a narcotic effect. Prolonged inhalation of moderate concentrations may cause nausea, vomiting, headache and drowsiness. Chronic overexposure may result in lung/respiratory, liver and or kidney damage, blood cell disorders, cardiovascular effects (ventricular fibrillation). Exposure to and/or consumption of alcohol may increase toxic effects. A common air contaminant. A food additive permitted in food for human consumption. Reported as carcinogenic. [51],[107],[56],[55],[98]

**Toxicity:** Moderate.

TWA: 50 ppm (270 mg/m<sup>3</sup>) [1]  
 STEL: 200 ppm (1080 mg/m<sup>3</sup>) [1]  
 CL: 150 ppm (800 mg/m<sup>3</sup>) for 10 min [51]  
 IDLH: 1000 ppm (5375 mg/m<sup>3</sup>) [107],[56]  
 Peak: 300 ppm (1610 mg/m<sup>3</sup>) for 15 min in any 2 hr period [51]  
 Odor threshold: 18-72 ppm (100-400 mg/m<sup>3</sup>) -- recognition [104]  
 50 ppm (270 mg/m<sup>3</sup>) [107]  
 Carcinogenicity: animal positive [22],[51],[35]  
 positive in mice, negative in rats [26],[40]  
 determined to be carcinogenic in 1976 by National  
 Cancer Institute [5]  
 Mutagenicity: equivalent tumorigenic agent [55]  
 positive [9]

**Exposure:**

External:

Non-Lethal: 160 ppm (860 mg/m<sup>3</sup>) -- eye irritation [104]  
 Lethal: unknown

Oral:

Non-lethal: 812 mg/kg body wt -- liver and kidney damage [51]  
 Lethal dose: 7 g/kg body wt [51]

Inhalation:

Short-term Inhalation Limits: 200 ppm (1080 mg/m<sup>3</sup>) for 30 min [107]  
 Non-lethal: 110 ppm/8 hr -- skin, eye, mucous membrane irritation [51]  
 160 ppm (860 mg/m<sup>3</sup>) for 83 min -- CNS effects [51]  
 400 ppm (2150 mg/m<sup>3</sup>) -- generally unsatisfactory [104]  
 800 ppm (4300 mg/m<sup>3</sup>) -- symptoms of illness [104]  
 2000 ppm (10,750 mg/m<sup>3</sup>) -- severe toxic effects [104]  
 2500-6500 ppm (13-35 g/m<sup>3</sup>) -- full narcosis [104]  
 1280 ppm (6900 mg/m<sup>3</sup>) for 10 min -- CNS effects [51]  
 Lethal: 2900 ppm (15,600 mg/m<sup>3</sup>) [51]

## 472 - Trichlorofluoromethane

Trichlorofluoromethane

CCl<sub>3</sub>F

CAS RN: 75-69-4

Syn: Trichlorofluoromethane \* Methane, trichlorofluoro- \* Algofrene type 1  
 \* Arcton 9 \* Electro-CF 11 \* Eskimon 11 \* F-11 \* F 11B \* FC 11 (halocarbon)  
 \* FKW 11 \* Fluorocarbon no. 11 \* Fluorochloroform \* Fluorotrichloromethane  
 \* Freon 11 \* Freon 11A \* Freon 11B \* Freon HE \* Freon MF \* Frigen 11 \*  
 Frigen 11A \* Genetron 11 \* Halocarbon 11 \* Isceon 11 \* Isceon 131 \* Isotron  
 11 \* Kaltron 11 \* Ledon 11 \* Methane, fluorotrichloro- \*  
 Monofluorotrichloromethane \* NCI-C04637 \* Propellant 11 \* R 11  
 (refrigerant) \* R 11 (halocarbon) \* RCRA Waste Number U121 \* Refrigerant 11  
 \* Trichloromonofluoromethane \* Ucon 11 \* Ucon fluorocarbon 11 \* Ucon  
 refrigerant 11 \*

Molecular formula: CCl<sub>3</sub>F

Mixed Halogenated Aliphatic Halide

## Physical properties:

Relative molecular mass:	137.368	
Specific gravity:	1.494 @ 17°C	[104], [22]
	1.494 @ 17.2°C	[108]
	1.485 @ 21°C	[10]
	1.484 @ 17.2°C	[47], [51]
	1.467 @ 25°C	[105]
Boiling point:	24.9°C	[47]
	24.1°C	[51]
	24.°C	[56]
	23.9°C	[107]
	23.8°C	[10], [104]
	23.82°C	[105]
	23.7°C	[22], [108]
	23.77°C	[7]
	23.65°C	[48]
	23.63°C	[49]
Melting point:	-110.48°C	[49]
	-111.°C	[10], [51], [104], [105], [108], [48]
Refractive index:	1.3824	[49]
	1.374 @ 25°C	[105]
Vapor pressure:	53.3 kPa @ 6.8°C (400mm)	[47], [105], [20]
	91.598 @ 20°C (687mm)	[104]
	105.6 @ 25°C (792mm)	[41]
	107.0 @ 25°C (802.8mm)	[24]
	130.7 @ 30°C (980mm)	[41]
Vapor density:	4.74	[41]
Evaporation rate:	unknown	
Relative dielectric permittivity:	2.303 @ 20°C	[49]
	2.28 @ 29°C	[105], [7]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.08653 W/(m-K) @ 25°C (liq)	[105]
	0.00837 @ 25°C (gas)	[105]
Electrical resistivity:	unknown	
Critical temperature:	198.0°C	[47], [49], [10], [105], [7], [48]
Critical pressure:	4.38 MPa	[10], [22], [108], [7]
	4.41	[49], [105]
	4.46	[48]



Dynamic viscosity:	0.42 mPa-s @ 25°C	[105]
	0.405 @ 30°C	[7]
Kinematic viscosity:	0.282 $\mu\text{m}^2/\text{s}$ @ 25°C	
	0.271 @ 30°C	
Surface tension:	19.09 mN/m @ 15°C	[49]
	18. @ 25°C	[49], [105]
	19. @ 25°C	[7]
Contact angle:	unknown	
Thermal expansion coefficient:	unknown	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	1.50x10 <sup>-30</sup> C-m	[105], [108]
	1.53x10 <sup>-30</sup> C-m (gas)	[49]
Ionization potential:	11.77 eV (PI)	[105]
Magnetic volume susceptibility:	-8.02 SI units @ 17°C	[105]
Speed of sound:	unknown	
Heat of melting:	6.895 kJ/mol	[49]
	6.901	[7]
Heat of vaporization:	25.02 kJ/mol	[7]
	25.06	[49]
	24.79 @ bp	[105]
Heat of sublimation:	unknown	
Heat capacity @ 25°C:	0.12155 kJ/(mol-K) (liq)	[49], [105]
	0.07812 (gas)	[10], [105]
Heat of combustion:	unknown	
Heat of formation:	-301.53 kJ/mol @ 25°C (liq)	[20], [105]
	-301.33 (liq)	[49]
	-285.1 (gas)	[10]
	-284.9 (gas)	[49]
	-284.7 (gas)	[7]
	-276.3 (gas)	[20], [105]
Gibbs (free) energy:	-237.01 kJ/mol @ 25°C (liq)	[105]
	-239.0 (gas)	[105]
	-245.68 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	2.53	[8], [21], [31], [41], [24]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	[31]
pK <sub>BH</sub> =	NA	
Henry's law constant =	11. kPa-m <sup>3</sup> /mol	[41]
	0.591	[41]
	9.83 @ 25°C	[24]
	175. @ 25°C	[24]
Hydrolysis half-life =	NA	[8]
Electrochemical data:	Unknown	
Clay-organic interaction data:	Unknown	
Solubility:	Slightly soluble in water. Miscible with ethanol and ether.	
	[47], [108], [49], [104],	
	0.11 wt% in water @ 25°C	[49], [105]
	0.108 wt% in water @ 30°C	[24]

#### 474 - Trichlorofluoromethane

**Form:** Colorless, nonflammable, volatile liquid or gas. Odorless in concentrations of less than 20% (by volume air); in higher concentrations, its odor is mild and somewhat ethereal chlorinated solvent odor, similar to that of carbon tetrachloride. [51],[7],[22]

**Use:** Manufacture of aerosol sprays, commercial refrigeration equipment, cleaning compounds; solvent; fire extinguisher; blowing agent for polyurethane foams; chemical intermediate; organic synthesis. [56],[22],[104],[41]

**Fire and explosion hazard:** Very low.

Flash point: NA

l<sub>el</sub>: NA

Autoign. temp.: NA

Nonflammable liquid. Produces irritating and highly toxic fumes of CO, CO<sub>2</sub>, hydrogen chloride gas, phosgene gas, hydrogen fluoride when heated to decomposition. Use water spray or fog nozzle to keep cylinder cool. Move cylinder away from fire if there is no risk. [51],[108],[55]

**Incompatibility:** Chemically active metals such as sodium, potassium, magnesium, aluminum, zinc, calcium, lithium, copper, bronze, silver, beryllium, alkali and alkaline earth metals. [56],[51],[55]

**Handling:** Avoid heat and flame. Avoid breathing vapor or mist (appropriate respirator or self-contained breathing apparatus). Avoid repeated or prolonged contact with eyes, skin, or clothing (leather gloves; safety goggles). Use in a well-ventilated area (fume hood). Safety shower and eye bath should be provided. Keep container tightly closed. Contents under pressure. Refrigerate. [7],[57],[55]

**Health effects:** Trichlorofluoromethane is a slight irritant. Routes of entry are inhalation, ingestion, or skin absorption. Points of attack include skin, eyes, respiratory system. Comparatively little toxicity in low concentrations. Inhalation may cause nausea, dizziness, headache, or difficult breathing. It can cause rapid suffocation. May cause frostbite. Exposure to high concentrations of vapor may cause light-headedness, disorientation, nausea, vomiting, narcosis, cardiac dysrhythmias, hypotension and death. The cardiac dysrhythmias are potentially lethal because of sensitization of the myocardium to endogenous epinephrine. [7],[107],[51],[56],[55]

**Toxicity:** Low

TWA: no value set [1]

STEL: no value set [1]

CL: 1000 ppm (5600 mg/m<sup>3</sup>) [1]

IDLH: 10000 ppm (56 g/m<sup>3</sup>) [56]

Peak: unknown

Odor threshold: 5-209 ppm (28-1175 mg/m<sup>3</sup>) [104]

200000 ppm (1100 g/m<sup>3</sup>) (20 vol%) [107]

Carcinogenicity: not conclusive; indefinite with rats; negative in mice [51],[104]

negative in small animals [36]

Mutagenicity: nonmutagenic in small animals [30]

**Exposure:**

**External:**

Non-lethal: unknown

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: unknown

**Inhalation:**

Short-term Inhalation Limits: unknown

Non-lethal: 3000-10000 ppm (16.8-56 g/m<sup>3</sup>) inhaled is exhaled entirely  
after 3-5 min [7]

50000 ppm (280 g/m<sup>3</sup>) for 30 min -- eye irritation,  
peripheral nervous system effects [104]

100000 ppm (560 g/m<sup>3</sup>) for 2 hr -- toxic effects [7]

Lethal: unknown

## 476 - 2,4,6-Trichlorophenol

2,4,6-Trichlorophenol

 $C_6H_3Cl_3O$ 

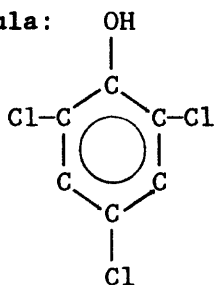
CAS RN: 88-06-2

Syn: 2,4,6-Trichlorophenol \* Phenol, 2,4,6-trichloro- \* Dowside 2S \*  
 Dowside 25 \* Dowicide 2S \* NCI-C02904 \* Omal \* Phenachlor \* RCRA Waste  
 Number U231 \* RCRA Waste Number F027 \* 2,4,6-TCP \* 2,4,6-TCP-Dowicide 25 UN  
 2020 (dot) \*

Molecular formula:  $C_6H_2Cl_3OH$ 

Polychlorinated Phenol

Structural formula:



## Physical properties:

Relative molecular mass:	197.448	
Specific gravity:	1.675	[22]
	1.490 (75/4)	[104], [105], [10], [51], [47]
Boiling point:	248.°-249°C	[22]
	246.°C	[105], [108], [10], [47]
	244.5°C	[104], [51]
Melting point:	69.5°C	[105], [56]
	69.°C	[10], [108]
	68.°-69°C	[47]
	68.5°C	[105]
	68.°C	[104], [51]
	62.°C (fp)	[51]
	61.°C (fp)	[22]
Refractive index:	NA	
Vapor pressure:	3.3x10 <sup>-4</sup> kPa @ 8°C	(0.0025mm) [41]
	0.0011 @ 24°C	(0.0084mm) [23]
	0.133 @ 76.5°C	(1mm) [51], [105]
	1.33 @ 120.2°C	(10mm) [105]
Vapor density:	NA	
Evaporation rate:	NA	
Relative dielectric permittivity:	unknown	
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	NA	
Kinematic viscosity:	NA	
Surface tension:	NA	
Contact angle:	NA	
Thermal expansion coefficient:	unknown	
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	



#### 478 - 2,4,6-Trichlorophenol

**Incompatibility:** Acid chlorides; acid anhydrides; oxidizing agents. [55]

**Handling:** Avoid heat and flame. Prevent inhalation of dust, mist, or vapor (appropriate respirator or self-contained breathing apparatus). Prevent contact with skin and eyes (resistant gloves, safety goggles, other protective clothing). Avoid prolonged or repeated exposure. Readily absorbed through skin. Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry, secure poison area or cabinet. [55]

**Health effects:** 2,4,6-TCP is an irritant and suspected carcinogen. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include skin, eyes, respiratory system. It is irritating to eyes, skin, mucous membranes and upper respiratory tract. Prolonged contact can cause damage to the eyes. Effects may vary from mild irritation to severe destruction of tissue depending on the intensity and duration of exposure. Chronic overexposure may cause cancer or alter genetic material. [51],[22],[55],[99]

**Toxicity:** Low.

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: 0.0001-0.0003 ppm (0.0010-0.0021 mg/m<sup>3</sup>) [104]

Carcinogenicity: results positive in mice and rats [51],[56]  
                  limited human evidence [55]

Mutagenicity: indefinite [99]  
                  positive [37],[58]

**Exposure:** Unknown

Vinyl chloride

 $C_2H_3Cl$ 

CAS RN: 75-01-4

Syn: Vinyl chloride \* Ethene, chloro- \* Chloroethene \* 1-Chloroethene \* Chloroethylene \* Chloroethylene \* 1-Chloroethylene \* Ethylene, chloro- \* Ethylene monochloride \* Monochloroethene \* Monochloroethylene \* MVC \* RCRA Waste Number U043 \* Trovidur \* UN 1086 (DOT) \* VCL \* VCM \* Vinyl chloride monomer \* Vinyl C monomer \*

Molecular formula:  $CH_2=CH-Cl$ 

Monochlorinated Aliphatic Hydrocarbon

**Physical properties:**

Relative molecular mass:	62.4988	
Specific gravity:	0.9195 (15/4)	[51]
	0.9121 (15/4)	[104]
	0.9121 (20/20)	[22]
	0.9106	[106], [105], [108]
	0.969 @ -13°C	[107]
	0.97 @ -14°C	[10]
	0.9834 (-20/4)	[15], [7]
Boiling point:	-12.°C	[47]
	-13.37°C	[105], [108]
	-13.4°C	[106]
	-13.80°C	[107], [49]
	-13.9°C	[10], [22], [51], [104], [7]
	-14.°C	[56]
Melting point:	-153.°C	[104]
	-153.79°C	[49]
	-153.8°C	[106], [105], [107], [108]
	-159.7°C	[10], [22], [7]
	-160.°C	[47], [51]
	-161.°C	[104]
Refractive index:	1.3682	[49]
	1.3700	[106], [105], [108]
Vapor pressure:	32.00 kPa @ -40°C (240mm)	[104]
	53.32 @ -28°C (400mm)	[105], [7]
	77.33 @ -20°C (580mm)	[104]
	254.33 @ 10°C (1908mm)	[7]
	306.6 @ 20°C (2300mm)	[22]
	337.3 @ 20°C (2530mm)	[108]
	343.5 @ 20°C (2576mm)	[7]
	354.6 @ 25°C (2660mm)	[49], [104], [23]
	346.6 @ 25°C (2600mm)	[51]
	466.09 @ 30°C (3496mm)	[7]
Vapor density:	2.15	[104], [51]
	2.2	[107]
Evaporation rate:	unknown	
Relative dielectric permittivity:	6.26 @ 17.2°C (under pressure)	[49], [7]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	NA	
Critical temperature:	156.2°C	[15]
	156.5°C	[49]
	158.4°C	[107], [7]

# 480 - Vinyl chloride

Critical pressure:	5.6 MPa	[49], [15]
	5.34	[107], [7]
Dynamic viscosity:	0.328 mPa-s @ -40°C	
(calculated from	0.298 @ -30°C	
kinematic viscosity)	0.273 @ -20°C	
	0.252 @ -10°C	
Kinematic viscosity:	0.3339 $\mu\text{m}^2/\text{s}$ @ -40°C	[15]
	0.3026 @ -30°C	[15]
	0.2780 @ -20°C	[15], [7]
	0.2563 @ -10°C	[15]
Surface tension:	23.87 mN/m @ -30°C	[15]
	22.27 @ -20°C	[49], [15], [7]
	20.88 @ -10°C	[49], [15]
	16.0 @ 25°C	[107]
Contact angle:	unknown	
Thermal expansion coefficient:	NA	
Compressibility:	unknown	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	4.837x10 <sup>-30</sup> C-m	[105]
	4.34x10 <sup>-30</sup>	[49]
Ionization potential:	9.996 eV (S,PI)	[105]
Magnetic volume susceptibility:	-6.64x10 <sup>-6</sup> SI unit (liq @ 15°C)	[105]
Speed of sound:	unknown	
Heat of melting:	4.747 kJ/mol	[105], [107], [15]
	4.745	[49]
Heat of vaporization:	20.811 kJ/mol	[15]
	20.799	[49]
	23.12	[107]
	26.222	[105]
Heat of sublimation:	unknown	
Heat capacity @ 27°C:	0.08983 kJ/(mol-K) (gas)	[49]
@ 25°C:	0.05376 (gas)	[10], [105]
Heat of combustion:	-1249.8 kJ/mol @ 25°C (gas)	[49]
	-1181.9 (gas)	[107]
Heat of formation:	14.6 kJ/mol @ 25°C (liq)	[49], [105]
	33.77 (gas)	[49]
	35.59 (gas)	[10], [105]
Gibbs (free) energy:	51.92 kJ/mol @ 25°C (gas)	[10], [105]
Analytical chemistry: pP <sub>oct</sub> =	1.38	[23], [100]
	1.23	[31]
	0.60	[8], [41]
pK <sub>s</sub> =	NA	
pK <sub>a</sub> =	NA	
pK <sub>BH</sub> =	NA	
Henry's law constant =	282. kPa-m <sup>3</sup> /mol	[41]
	240.	[41]
	2.23	[41]
	124. @ 10°C	[41]
	5.67 @ 25°C	[41]
Hydrolysis half-life =	3.0x10 <sup>8</sup> sec	[8]

Electrochemical data: Unknown



**Clay-organic interaction data:** Unknown

**Solubility:** Slightly soluble in water. Soluble in ethanol, carbon tetrachloride, benzene. Very soluble in ether. [10],[108],[104],[49]

0.0060 wt% in water @ 10°C [41]

0.95 wt% in water @ 15°C [41]

0.11 wt% in water @ 25°C [104]

0.27 wt% in water @ 25°C [49],[23]

**Form:** Colorless gas or liquid. Faintly sweet odor. Polymerizes in the presence of air sunlight, heat or catalyst. It is shipped in steel cylinders as a liquefied gas under its own pressure. It is shipped with an inhibitor (phenol) to prevent polymerization. [51],[108],[22]

**Use:** Refrigerant; in organic syntheses; vinyl monomer in production of polyvinyl chloride (PVC) and copolymers; adhesives for plastics. 19th highest volume chemical produced in U.S. (1979). [108],[56],[22]

**Fire and explosion hazard:** Very high.

Flash point: (CC) -78°C [108]

(OC) -77.8°C [22]

(OC) -78°C [49]

(OC) -78.9°C [107]

uel: 26% [107]

22% [51]

lel: 4% [107]

3.6% [51]

Autoign. temp.: 472°C [22],[51],[107],[7]

Extremely flammable gas; severe explosion risk at concentrations of 30000 ppm. Dangerous fire hazard when exposed to heat, flame or oxidizers. Large fires of this material are practically inextinguishable. Flashback may occur along vapor trail. Severe explosion hazard, in the form of vapor, when exposed to heat or flame. Also, on standing, forms peroxides in air and can then explode. Very dangerous when heated to decomposition as it emits highly toxic fumes of phosgene, hydrogen chloride and CO. Fight large fires by stopping the flow of gas and quickly removing the storage cylinder away from the area. For small fires use dry chemical powder or CO<sub>2</sub>. [51],[107],[22]

**Incompatibility:** Air. [51],[107]

**Handling:** WARNING: contact with the skin or by inhalation is prohibited. Before storing or handling this material, instructions for its use should be obtained from the supplier. Keep away from heat, flame, sources of ignition and air. Appropriate respirator or self-contained breathing apparatus required. Prevent skin contact (PVA coated nylon gloves and boots; protective overclothing; gas-tight goggles). Use in well-ventilated area (fume hood). Monitoring program is required for all vinyl chloride operations. [51],[57],[53],[56],[107],[7]

## 482 - Vinyl chloride

**Health effects:** Vinyl chloride is an irritant, central nervous system depressant, and human carcinogen. Routes of entry include absorption by inhalation, and eye and skin contact. Points of attack include liver, brain, and hemato-lymphopoietic system. It is an irritant to eyes, skin and mucous membranes. Liquid on contact with the skin, may cause severe skin irritation, frost bite and burns. It causes skin burns by rapid evaporation and consequent freezing. In high concentrations, it acts as an anesthetic. Chronic exposure has shown liver injury in rats and rabbits. Circulatory and bone changes in the fingertips reported in workers handling unpolymerized materials. Causes "vinyl chloride disease". May be narcotic in high concentrations. It is reported to cause cancer in the liver, lung, brain, and kidneys. [104],[108],[51],[56],[100]

**Toxicity:** High.

TWA: 5 ppm (10 mg/m<sup>3</sup>) [1]

STEL: no value set [1]

CL: 5 ppm (13 mg/m<sup>3</sup>) over any 15 minute period [51],[56]

IDLH: unknown

Peak: unknown

Odor threshold: 10-20 ppm (26-52 mg/m<sup>3</sup>) [104]

25000 ppm (64 g/m<sup>3</sup>) [104]

260 ppm (100 mg/m<sup>3</sup>) [107]

Carcinogenicity: confirmed human carcinogen [49],[51],[56],[104],[1]

Mutagenicity: weakly mutagenic in *Salmonella* test (without liver homogenate) [104]  
positive [30]

**Exposure:**

External:

Non-lethal: unknown

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: unknown

Inhalation:

Short-term Inhalation Limits: 500 ppm (1280 mg/m<sup>3</sup>) for 5 min [107]

Non-lethal: 500 ppm for 4 yr at intervals -- carcinogenic effects [51]

1000 ppm (2560 mg/m<sup>3</sup>) -- slowly produces mild disturbances such as drowsiness, blurred vision, staggering gait, tingling and numbness in feet and hands [7]

25000 ppm (64 g/m<sup>3</sup>) -- dizziness, disorientation, and a burning sensation in the soles of the feet [104]

70000 to 100000 ppm (179-256 g/m<sup>3</sup>) -- causes narcosis [7]

Lethal: 120000 ppm (307 g/m<sup>3</sup>) -- may be dangerous to life [7]

Water

H<sub>2</sub>O

CAS RN: 7732-18-5

Syn: Water \* Dihydrogen oxide \* Distilled water \* Ice \* Water vapor \*Molecular formula: H<sub>2</sub>O

Inorganic

## Physical properties:

Relative molecular mass:	18.01528		
Specific gravity:	1.000		[definition]
Boiling point:	0.0°C		[definition]
Melting point:	100.0°C		[definition]
Refractive index:	1.33299		[105]
Vapor pressure:	0.1333 kPa @ -17.3°C (1mm)		[105]
	1.333 @ 11.3°C (10mm)		[105]
	2.3378 @ 20°C (17.5mm)		[105]
	5.3329 @ 34.1°C (40mm)		[105]
	13.332 @ 51.6°C (100mm)		[105]
	53.329 @ 83.0°C (400mm)		[105]
	101.327 @ 100°C (760mm)		[105]
Vapor density:	unknown		
Evaporation rate:	unknown		
Relative dielectric permittivity:	89.02 @ 0°C		[39]
	87.90 @ 0°C		[105]
	85.90 @ 5°C		[105]
	85.82 @ 5°C		[39]
	84.24 @ 10°C		[39]
	83.95 @ 10°C		[105]
	82.04 @ 15°C		[105]
	81.98 @ 15°C		[39]
	80.50 @ 20°C		[39]
	80.18 @ 20°C		[105]
	79.20 @ 25°C		[39]
	78.36 @ 25°C		[105]
	77.16 @ 30°C		[39]
	76.58 @ 30°C		[105]
	73.15 @ 40°C		[105]
	69.88 @ 50°C		[105]
	66.76 @ 60°C		[105]
	63.78 @ 70°C		[105]
	60.93 @ 80°C		[105]
	58.20 @ 90°C		[105]
	55.58 @ 100°C		[105]
Loss tangent:	unknown		
Relaxation time:	17.71x10 <sup>-12</sup> sec @ 0°C		[39]
	14.42 @ 5°C		[39]
	12.48 @ 10°C		[39]
	10.51 @ 15°C		[39]
	9.27 @ 20°C		[39]
	8.33 @ 25°C		[39]
	7.93 @ 30°C		[39]
Thermal conductivity:	0.5552 W/(m-K) @ -3°C		[105]
	0.5744 @ 7°C		[105]
	0.6096 @ 27°C		[105]
	0.611 @ 30°C		[49]

# 484 - Water

	0.6372	@ 47°C	[105]
	0.6594	@ 67°C	[105]
	0.6804	@ 97°C	[105]
Electrical resistivity:	0.303 MOhm-m	@ 15°C	[49]
	0.256	@ 18°C	[49]
	0.227	@ 20°C	[49]
	0.170	@ 25°C	[49]
	0.129	@ 30°C	[49]
Critical temperature:	374.1°C		[105]
Critical pressure:	22.12 MPa		[105]
Dynamic viscosity:	1.787 mPa-s	@ 0°C	[105]
(kinematic viscosity	1.307	@ 10°C	[105]
values are the same)	1.002	@ 20°C	[105]
	0.8904	@ 25°C	[105]
	0.7975	@ 30°C	[105]
	0.6529	@ 40°C	[105]
	0.5468	@ 50°C	[105]
	0.4665	@ 60°C	[105]
	0.4042	@ 70°C	[105]
	0.3547	@ 80°C	[105]
	0.3147	@ 90°C	[105]
	0.2818	@ 100°C	[105]
Surface tension:	75.60 mN/m	@ 0°C	[105]
	74.22	@ 10°C	[105]
	72.75	@ 20°C	[105]
	71.97	@ 25°C	[105]
	71.18	@ 30°C	[105]
	69.56	@ 40°C	[105]
	67.91	@ 50°C	[105]
	66.18	@ 60°C	[105]
	64.4	@ 70°C	[105]
	62.6	@ 80°C	[105]
	58.9	@ 100°C	[105]
Contact angle: [18]			
	sessile	advancing	receding
quartz	29	39	8
calcite	40	46	6
biotite	9	11	0
Ca-mont.	22	swelled	swelled
Thermal expansion coefficient:	0.00020661 K <sup>-1</sup>	@ 20°C	[49]
	0.00025705	@ 25°C	[49]
	0.00030314	@ 30°C	[49]

Compressibility:	0.501 nPa <sup>-1</sup> @ 0°C	[105]
	0.478 @ 10°C	[105]
	0.458 @ 20°C	[105]
	0.457 @ 25°C	[105]
	0.446 @ 30°C	[105]
	0.441 @ 40°C	[105]
	0.440 @ 50°C	[105]
	0.443 @ 60°C	[105]
	0.449 @ 70°C	[105]
	0.457 @ 80°C	[105]
	0.468 @ 90°C	[105]
	0.480 @ 100°C	[105]
Vapor diffusivity:	22.0 μm <sup>2</sup> /s @ 0°C	[104]
Solution diffusivity:	0.21 nm <sup>2</sup> /s in glycerol	[104]
Electric dipole moment:	6.17x10 <sup>-30</sup> C-m	[105]
Ionization potential:	12.6 eV (PI)	[105]
Magnetic volume susceptibility:	-154.7x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	1496.7 m/s @ 25°C	[105]
Heat of melting:	6.012 kJ/mol	[10]
Heat of vaporization:	40.68 kJ/mol	[10]
Heat of sublimation:	50.982 kJ/mol	[49]
Heat capacity @ 25°C:	0.075342 kJ/(mol-K) (liq)	[10]
	0.03360 (gas)	[10]
Heat of combustion:	NA	
Heat of formation:	-286.02 kJ/mol @ 25°C (liq)	[10]
	-241.98 (gas)	[10]
Gibbs (free) energy:	-237.34 kJ/mol @ 25°C (liq)	[10]
	-228.74 (gas)	[10]
Analytical chemistry:	pP <sub>oct</sub> = NA	
	pK <sub>s</sub> = NA	
	pK <sub>a</sub> = NA	
	pK <sub>BH</sub> = NA	
	pK <sub>w</sub> = 14.9435 @ 0°C	[105]
	14.5346 @ 10°C	[105]
	14.1669 @ 20°C	[105]
	13.9965 @ 25°C	[105]
	13.883 @ 30°C	[105]
	13.542 @ 40°C	[49]
	13.272 @ 50°C	[49]
Henry's law constant =	NA	
Hydrolysis half-life =	NA	
Electrochemical data:	any electrochemistry text	

**Clay-organic interaction data:** Water is not an organic compound, but it does have an intimate association with clay minerals, their formation and occurrence, and participates with clays in many active processes and interactions. The presence of water frequently modifies clay-organic interactions (Mortland, 1970; Rausell-Colom and Serratosa, 1987; [18]). For general reference, see Elprince, 1986; Greenland and Hayes, 1981; Newman, 1987; Sposito, 1984; van Olphen, 1977; Yariv and Cross, 1979.

**Solubility:** Miscible with acetic acid, acetone, 1,4-dioxane, ethanol, methanol, and most ionic organic chemicals. [105],[49]

**486 - Water**

**Form:** Clear, colorless liquid. No odor. No taste. [22]

**Use:** Universal solvent except for non-ionic organic chemicals. [22]

**Fire and explosion hazard:** None.  
Not combustible.

**Incompatibility:** 1,1,1-Trichloroethane, alkali metals, alkaline earths.

**Handling:** No special precautions. Keep container tightly closed.  
Suitable for any general chemical storage.

**Health effects:** Harmless under normal situations.

**Toxicity:** None

**Exposure:** None

m-Xylene

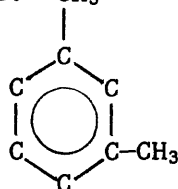
C<sub>8</sub>H<sub>10</sub>

CAS RN: 108-38-3

Syn: m-Xylene \* Benzene, 1,3-dimethyl- \* 1,3-Dimethylbenzene \* m-Dimethylbenzene \* m-Methyltoluene \* UN 1307 (DOT) \* 1,3-Xylene \* 3-Xylene \* meta-Xylene \* m-Xylol \* Xylol \*

Molecular formula: m-C<sub>6</sub>H<sub>4</sub>(CH<sub>3</sub>)<sub>2</sub>

Monocyclic Aromatic Hydrocarbon

Structural formula: CH<sub>3</sub>**Physical properties:**

Relative molecular mass:	106.1674	
Specific gravity:	0.86417	[14]
	0.86436	[49]
	0.8642	[10], [105]
	0.864	[104], [107], [51]
Boiling point:	138.8°C	[22]
	139.103°C	[14]
	139.12°C	[49]
	139.1°C	[10], [107], [106], [105]
	139.°C	[104], [51]
Melting point:	-47.4°C	[22]
	-47.87°C	[105]
	-47.872°C	[49]
	-47.9°C	[10], [106], [107], [51]
	-48.°C	[104]
	-53.°C	[104]
Refractive index:	1.4972	[10], [105]
	1.49722	[14], [49]
	1.4973	[22]
Vapor pressure:	0.133 kPa @ -6.9°C (1mm)	[107]
	0.80 @ 20°C (6mm)	[104]
	1.20 @ 20°C (9mm)	[32]
	1.11 @ 25°C (8.3mm)	[49]
	1.115 @ 25°C (8.363mm)	[14]
	1.33 @ 28.3°C (10mm)	[107], [51]
	1.46 @ 30°C (11mm)	[104]
Vapor density:	3.66	[104], [51]
Evaporation rate:	0.7	[32]
Relative dielectric permittivity:	2.3742 @ 20°C	[49], [105], [11]
	2.242 @ 25°C	[14]
	2.25 @ 30°C	[11]
	2.3503 @ 30°C	[2]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.1362 W/(m-K) @ 0°C	[10]
	0.156 @ 20°C	[47]
	0.145 @ 20°C	[48]
	0.1577 @ 25°C	[105]

# 488 - *m*-Xylene

Electrical resistivity:	1.16x10 <sup>7</sup> MOhm-m	[49]
Critical temperature:	346.°C	[105], [48]
	343.90°C	[49]
	343.82°C	[10]
	343.8°C	[107]
Critical pressure:	3.58 MPa	[48]
	3.541	[10]
	3.54	[107]
	3.536	[49]
	3.516	[105]
Dynamic viscosity:	0.806 mPa-s @ 0°C	[105]
	0.714 @ 10°C	[48]
	0.650 @ 15°C	[105]
	0.622 @ 20°C	[48]
	0.617 @ 20°C	[10]
	0.620 @ 20°C	[105]
	0.581 @ 25°C	[49]
	0.561 @ 30°C	[48]
	0.497 @ 40°C	[105]
Kinematic viscosity:	0.933 μm <sup>2</sup> /s @ 0°C	
	0.826 @ 10°C	
	0.752 @ 15°C	
	0.720 @ 20°C	
	0.714 @ 20°C	
	0.717 @ 20°C	
	0.672 @ 25°C	
	0.649 @ 30°C	
	0.575 @ 40°C	
Surface tension:	33.438 mN/m @ -20°C	[10]
([10] values are calculated)	32.334 @ -10°C	[10]
	31.230 @ 0°C	[10]
	30.126 @ 10°C	[10]
	28.6 @ 20°C	[107]
	28.63 @ 20°C	[14]
	28.66 @ 20°C	[49]
	28.9 @ 20°C	[105]
	29.022 @ 20°C	[10]
	28.10 @ 25°C	[49]
	27.54 @ 30°C	[14]
	27.918 @ 30°C	[10]
	26.44 @ 40°C	[14]
	26.814 @ 40°C	[10]
	25.710 @ 50°C	[10]
	24.606 @ 60°C	[10]
	23.502 @ 70°C	[10]
	22.398 @ 80°C	[10]
	21.294 @ 90°C	[10]
	20.190 @ 100°C	[10]

Contact angle: [18]

	sessile	advancing	receding
quartz	6	7	3
calcite	8	14	5
biotite	11	10	3
Ca-mont.	swelled	swelled	swelled



Thermal expansion coefficient.:	0.000981 K <sup>-1</sup>	[49]
	0.00099	[48]
Compressibility:	0.744 nPa <sup>-1</sup> @ 0°C	[105]
	0.794 @ 10°C	[105]
	0.846 @ 20°C	[105]
	0.8621 @ 25°C	[49]
	0.903 @ 30°C	[105]
	0.963 @ 40°C	[105]
	1.025 @ 50°C	[105]
	1.101 @ 60°C	[105]
	1.177 @ 70°C	[105]
	1.256 @ 80°C	[105]
Vapor diffusivity:	6.9 μm <sup>2</sup> /s	[59]
Solution diffusivity:	0.71 nm <sup>2</sup> /s (calc)	[59]
Electric dipole moment:	1.234x10 <sup>-30</sup> C-m	[10]
Ionization potential:	8.58 eV (PI,PE)	[105]
Magnetic volume susceptibility:	-7.835x10 <sup>-6</sup> SI units @ 20°C	[105]
Speed of sound:	unknown	
Heat of melting:	11.6 kJ/mol	[10]
	11.569	[49]
	11.554	[105]
Heat of vaporization:	41.470 kJ/mol	[105]
	42.656 @ 25°C	[49]
	36.4	[107], [10]
	36.36 @ bp	[49]
Heat of sublimation:	42.71 kJ/mol	[10]
Heat capacity @ 25°C:	0.1834 kJ/(mol-K) (liq)	[10]
	0.18344 (liq)	[49]
	0.1818 (liq)	[105]
	0.1277 (gas)	[10]
Heat of combustion:	-4554.90 kJ/mol @ 25°C (liq)	[20]
	-4551.86 (liq)	[49]
	-4597.61 (gas)	[20]
	-4556.9 @ 20°C (liq)	[105]
Heat of formation:	-25.46 kJ/mol @ 25°C (liq)	[10]
	-25.418 (liq)	[49]
	17.258 (gas)	[10]
Gibbs (free) energy:	107.73 kJ/mol @ 25°C (liq)	[10]
	118.95 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	3.20 [104],[21],[27],[101],[24],[59]	
pK <sub>s</sub> =	unknown	
pK <sub>a</sub> =	unknown	
pK <sub>BH</sub> =	3.2 @ 0°C in HF	[49]
Henry's law constant =	0.778 kPa-m <sup>3</sup> /mol	[24]
	0.71	[41]
	0.64 @ 25°C	[41]
	0.314 dimensionless (calc)	[59]
Hydrolysis half-life =	unknown	

Electrochemical data: Neikam and Desmond (1964), Meites and Zuman (1977), Nyberg (1978)

## 490 - *m*-Xylene

**Clay-organic interaction data:** Xylene increases the hydraulic conductivity of clay soils (Anderson and Brown, 1981; Anderson and Jones, 1983; Anderson et al., 1981; Brown and Thomas, 1984; Brown et al., 1986; Lord et al., 1983; Rao et al., 1988; Schramm et al., 1986). Physical adsorption of xylenes and coordination to the exchangeable cations when intercalated by Cu(II)montmorillonite. Frequencies of C-C stretching and C-H out-of-plane vibrations of *m*-xylene in the liquid state and when adsorbed by Cu(II)-montmorillonite. (Theng, 1974). Also see [18] and Pinnavaia and Mortland (1971).

**Solubility:** Almost insoluble in water. Miscible with ethanol, ether, acetone, carbon tetrachloride, petroleum ether, benzene and many other organic solvents. [51],[32],[49],[108]

0.00003 wt%	in water @ 20°C	[32]
0.02	wt% in water @ 20°C	[10]
0.0146	wt% in water @ 25°C	[49],[101]

**Form:** Colorless liquid. Characteristic aromatic, sweet, benzene-like odor. [51],[107],[104],[32],[108]

**Use:** An intermediate during the manufacture of plastics, synthetics and mixed/pure isomers; as a dilutor or solvent in surface coatings, printing operations and manufacture of rubber; degreasing agent in plastics and electronics; solvent for alkyd resins, lacquers, enamels, rubber cements; in organic synthesis reactions and manufacture of epoxy resins; in formulation of insecticides; in manufacture of xylene-formaldehyde resins, pharmaceuticals, vitamins, leather, dyes and other organics; sterilizing agent for catgut; with Canadian balsam as oil-immersion in microscopy; cleaning agent in microscope techniques; raw material for production of benzoic acid, phthalic anhydride, isophthalic and terephthalic acids as well as their dimethyl esters used in the manufacture of polyester fibers; 12 wt% in aviation gasolines (high octane number). [56],[108],[104],[32]

**Fire and explosion hazard:** High.

Flash point: (CC) 28.9°C [107],[49]  
(OC) 23.2°C [14]

uel: 6.4% [107]

7.0% [51],[14]

lel: 1.1% [107],[51],[14]

Autoign. temp.: 530°C [107],[51]

Highly flammable liquid. Dangerous fire hazard when exposed to heat or flame. Flashback along vapor trail may occur. Moderate explosion hazard in the form of vapor when exposed to heat or flame. Vapor may explode if ignited in an enclosed area. When heated to decomposition it emits acrid smoke and toxic fumes or vapors (carbon monoxide, carbon dioxide). Contact with strong oxidizers may cause fires and explosions. Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder. Water may be ineffective. [51],[107]

**Incompatibility:** Strong oxidizing agents. [51]

**Handling:** Keep away from heat, sparks and flame. Avoid breathing vapor or mist (appropriate respirator or self-contained breathing apparatus). Avoid contact with eyes, skin or clothing (nitrile or PVA synthetic latex gloves and boots; safety goggles or face shield; lab coat, apron). Use with adequate ventilation (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Bond and ground containers when transferring liquid. Handle containers with nonsparking tools. Store in cool, dry, well-ventilated, flammable liquid storage area. [56],[57],[53],[32]

**Health effects:** Xylenes are moderately toxic. Routes of entry are inhalation of vapor, skin absorption, ingestion, and eye and skin contact. Points of attack include central nervous system, eyes, gastrointestinal tract, blood, liver, kidneys, and skin. Vapor or mist is irritating to the eyes, mucous membranes and upper respiratory tract. At high concentration, it may cause severe breathing difficulties (effects may be delayed), dizziness, staggering, drowsiness, unconsciousness, lung irritation, chest pain and edema which may be fatal. Also, breathing high concentrations may cause loss of appetite, nausea, vomiting and abdominal pain. Ingestion may cause nausea, vomiting, gastrointestinal irritation, headaches, blurred vision, dizziness and lowering of blood pressure. Repeated exposure of the eyes to high concentrations may cause reversible eye damage. Prolonged or repeated exposure may cause dermatitis. Chronic effects of overexposure may include kidney and/or liver damage and blood effects. Xylenes may be narcotic at high concentrations. Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. [32],[56],[51],[107],[55],[101]

**Toxicity:** Moderate.

TWA: 100 ppm (435 mg/m<sup>3</sup>) [1]

STEL: 150 ppm (655 mg/m<sup>3</sup>) [1]

CL: 200 ppm (870 mg/m<sup>3</sup>) averaged over 10 min period [51],[56]

IDLH: 10000 ppm (43.5 g/m<sup>3</sup>) [107],[56]

Peak: 300 ppm (1300 mg/m<sup>3</sup>) for 30 min duration [107]

Odor threshold: 0.3-170 ppm (1.3-740 mg/m<sup>3</sup>) -- detection [104]

0.5 ppm (2.1 mg/m<sup>3</sup>) [107]

Carcinogenicity: negative in small animals for mixed xylenes [25],[26]

Mutagenicity: not mutagenic [101]

**Exposure:**

External:

Non-lethal: 200 ppm (870 mg/m<sup>3</sup>) -- eye irritation, anorexia, nausea, vomiting, and abdominal pain [104]

200 ppm (870 mg/m<sup>3</sup>) -- eye irritant [107],[51]

Lethal: unknown

Oral:

Non-lethal: unknown

Lethal: 50 to 500 g/kg body wt. -- 50% chance of death [107]

Inhalation:

Short term Inhalation Limits: 300 ppm (1300 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: 98 ppm (424 mg/m<sup>3</sup>) for 6 hours for 6 days [51]

Lethal: unknown

## 492 - o-Xylene

o-Xylene

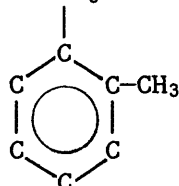
 $C_8H_{10}$ 

CAS RN: 95-47-6

Syn: o-Xylene \* Benzene, 1,2-dimethyl- \* 1,2-Dimethylbenzene \* o-Dimethylbenzene \* o-Methyltoluene \* UN 1307 (DOT) \* 1,2-Xylene \* 2-Xylene \* ortho-Xylene \* o-Xylol \*

Molecular formula:  $o-C_6H_4(CH_3)_2$ 

Monocyclic Aromatic Hydrocarbon

Structural formula:  $CH_3$ 

## Physical properties:

Relative molecular mass:	106.167	
Specific gravity:	0.8802	[10], [14], [105]
	0.880	[22], [104], [10], [107], [51]
Boiling point:	144.429°C	[49]
	144.411°C	[14]
	144.4°C	[104], [10], [107], [51], [105]
Melting point:	-25.2°C	[10], [107], [51]
	-25.182°C	[14], [49]
	-25.18°C	[105]
	-25.°C	[22], [104]
Refractive index:	1.5055	[105]
	1.50545	[14], [49]
	1.5054	[10]
Vapor pressure:	0.1333 kPa @ -3.8°C (1mm)	[105]
	0.666 @ 20°C (5mm)	[104]
	0.933 @ 20°C (7mm)	[32]
	0.880 @ 25°C (6.6mm)	[49]
	1.200 @ 30°C (9mm)	[104]
	1.333 @ 32.1°C (10mm)	[105]
	5.333 @ 59.5°C (40mm)	[105]
Vapor density:	3.7	[104], [32]
Evaporation rate:	0.7	[32]
Relative dielectric permittivity:	2.568 @ 20°C	[49], [105]
	2.57 @ 20°C	[10], [11]
	2.266 @ 20°C	[14]
	2.54 @ 30°C	[11]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	0.1442 W/(m-K) @ 0°C	[10]
	0.156 @ 20°C	[47]
	0.1055 @ 33°C	[10]
	0.1428 @ -20° - 80°C	[105]
Electrical resistivity:	$1.5 \times 10^7$ MOhm-m	[49]
Critical temperature:	359.°C	[105]
	357.18°C	[49]
	357.1°C	[10], [107]

Critical pressure:	3.734 MPa	[49]	
	3.733	[10]	
	3.62	[105]	
	3.372	[107]	
Dynamic viscosity:	1.122 mPa-s @ 0°C	[11]	
	1.105 @ 0°C	[105]	
	0.948 @ 10°C	[11]	
	0.876 @ 16°C	[105]	
	0.826 @ 20°C	[11]	
	0.820 @ 20°C	[105]	
	0.809 @ 20°C	[10]	
	0.756 @ 25°C	[49]	
	0.724 @ 30°C	[11]	
	0.627 @ 40°C	[105]	
Kinematic viscosity:	1.275 $\mu\text{m}^2/\text{s}$ @ 0°C		
	1.255 @ 0°C		
	1.077 @ 10°C		
	0.995 @ 16°C		
	0.939 @ 20°C		
	0.932 @ 20°C		
	0.919 @ 20°C		
	0.859 @ 25°C		
	0.823 @ 30°C		
	0.712 @ 40°C		
Surface tension:	34.712 mN/m @ -20°C	[10]	
(calculated in [10])	33.611 @ -10°C	[10]	
	32.510 @ 0°C	[10]	
	31.409 @ 10°C	[10]	
	30.53 @ 15.5°C	[107]	
	30.308 @ 20°C	[10]	
	30.10 @ 20°C	[105]	
	30.04 @ 20°C	[49]	
	29.49 @ 25°C	[49]	
	29.207 @ 30°C	[10]	
	28.106 @ 40°C	[10]	
	27.005 @ 50°C	[10]	
	25.904 @ 60°C	[10]	
	24.803 @ 70°C	[10]	
	23.702 @ 80°C	[10]	
	22.601 @ 90°C	[10]	
	21.500 @ 100°C	[10]	
Contact angle: [18]			
	sessile	advancing	receding
quartz	9	10	6
calcite	12	11	4
biotite	12	12	6
Ca-mont.	swelled	8	swelled
Thermal expansion coefficient:	0.000952 K <sup>-1</sup>	[49]	
Compressibility:	0.848 nPa <sup>-1</sup> @ 25°C	[49]	
Vapor diffusivity:	7.3 $\mu\text{m}^2/\text{s}$	[59]	
Solution diffusivity:	0.71 nm <sup>2</sup> /s (calc)	[59]	
Electric dipole moment:	2.07x10 <sup>-30</sup> C-m	[10], [105]	
	1.50x10 <sup>-30</sup>	[49]	

# 494 - o-Xylene

Ionization potential:	8.56 eV (PI)	[105]
Magnetic volume susceptibility:	-8.093x10 <sup>-6</sup> SI units @20°C	[105]
Speed of sound:	unknown	
Heat of melting:	13.62 kJ/mol	[107]
	13.61	[105]
	13.6	[10]
	13.598	[49]
Heat of vaporization:	41.862 kJ/mol	[105]
	43.434 @ 25°C	[49]
	36.82 @ bp	[49]
	36.8	[107], [10]
Heat of sublimation:	43.46 kJ/mol	[10]
Heat capacity @ 25°C:	0.188 kJ/(mol-K) (liq)	[10]
	0.18807 (liq)	[49]
	0.1876 (liq)	[105]
	0.1333 (gas)	[10]
Heat of combustion:	-4555.91 kJ/mol @ 25°C (liq)	[20]
	-4552.86 (liq)	[49]
	-4599.37 (gas)	[20]
	4570.73 @ 20°C (liq)	[105]
Heat of formation:	-24.451 kJ/mol @ 25°C (liq)	[10]
	-24.439 (liq)	[49]
	19.008 (gas)	[10]
Gibbs (free) energy:	110.4 kJ/mol @ 25°C (liq)	[10]
	122.2 (gas)	[10]
Analytical chemistry: pP <sub>oct</sub> =	3.12	[24], [59]
	2.95	[27]
	2.77	[104], [21], [101]
	2.77 - 3.16	[41]
	pK <sub>s</sub> unknown	
	pK <sub>a</sub> >15.	[59]
	pK <sub>BH</sub> = unknown	
Henry's law constant =	0.52 kPa-m <sup>3</sup> /mol	[24]
	0.534	[41]
	0.54 @ 25°C	[41]
	0.216 dimensionless	[59]
Hydrolysis half-life =	unknown	

Electrochemical data: Neikam and Desmond (1964), Meites and Zuman (1977), Nyberg (1978)

Clay-organic interaction data: Xylene increases the hydraulic conductivity of clay soils (Anderson and Brown, 1981; Anderson and Jones, 1983; Anderson et al., 1981; Brown and Thomas, 1984; Brown et al., 1986; Lord et al., 1983; Rao et al., 1988; Schramm et al., 1986). Physical adsorption of xylenes and coordination to the exchangeable cations when intercalated by Cu(II)montmorillonite. Frequencies of C-C stretching and C-H out-of-plane vibrations of o-xylene in the liquid state and when adsorbed by Cu(II)montmorillonite. (Theng, 1974). Also see [18] and Pinnavaia and Mortland (1971)

**Solubility:** Almost insoluble in water; miscible with absolute alcohol, ether, acetone, carbon tetrachloride, petroleum ether, benzene and many other organic solvents. [51],[32],[49],[104]

0.0175	wt% in water @ 25°C	[49]
0.0175	wt% in water @ 20°C	[104]
0.017	wt% in water @ 20°C	[10]
0.00003	wt% in water @ 20°C	[32]

**Form:** Colorless liquid. Sweet, characteristic benzene-like odor. [51],[107],[104]

**Use:** Intermediate during the manufacture of plastics, synthetics and mixed/pure isomers; dilutor or solvent in surface coatings, printing operations and manufacture of rubber; degreasing agent in plastics and electronics; solvent for alkyd resins, lacquers, enamels, rubber cements; in organic synthesis reactions and manufacture of epoxy resins; formulation of insecticides; manufacture of xylene-formaldehyde resins, pharmaceuticals, vitamins, leather, dyes and other organics; sterilizing agent for catgut; with Canadian balsam as oil-immersion in microscopy; cleaning agent in microscope techniques; raw material for production of benzoic acid, phthalic anhydride, isophthalic and terephthalic acids as well as their dimethyl esters used in the manufacture of polyester fibers; aviation gasolines. [56],[108],[22]

**Fire and explosion hazard:** High.

Flash point: (CC) 17.0°C [51]  
 (CC) 17.2°C [107]  
 (OC) 23.9°C [107]  
 (OC) 27.0°C [14]  
 (OC) 46.1°C [22]

uel: 7.0% [107]

6.0% [51]

lel: 1.1% [107]

1.0% [51]

Autoign. temp.: 465°C [107]

Highly flammable liquid. Dangerous fire hazard when exposed to heat or flame. Flashback along vapor trail may occur. Moderate explosion hazard in the form of vapor when exposed to heat or flame. Vapor may explode if ignited in an enclosed area. When heated to decomposition it emits acrid smoke and toxic fumes or vapors (CO, CO<sub>2</sub>). Contact with strong oxidizers may cause fires and explosions. Fight fire with alcohol or polymer foam, CO<sub>2</sub>, dry chemical powder. Water may be ineffective. [51],[107]

**Incompatibility:** Strong oxidizing agents. [51]

**Handling:** Keep away from heat, sparks and flame. Avoid breathing vapors or mist (appropriate respirator or self-contained breathing apparatus). Avoid contact with eyes, skin or clothing (nitrile or PVA synthetic latex gloves and boots; safety goggles or face shield, lab coat, apron). Use with adequate ventilation (fume hood). Safety shower and eye bath stations should be available. Keep container tightly closed. Bond and ground containers and use nonsparking tools when transferring liquid. Store in cool, dry, well-ventilated, flammable liquid storage area. [56],[57],[53],[32]

**Health effects:** Xylenes are moderately toxic. Routes of entry are inhalation of vapor slight percutaneous absorption of liquid, ingestion, and skin and eye contact. Points of attack include central nervous system, eyes, gastrointestinal tract, blood, liver, kidneys, and skin. Vapor or mist is irritating to the eyes, nose, mucous membranes and upper respiratory tract. At high concentration, it may cause severe breathing difficulties (effects may be delayed), dizziness, staggering, drowsiness, unconsciousness, lung irritation, chest pain and edema which may be fatal. Also, breathing high concentrations may cause loss of appetite, nausea, vomiting and abdominal pain. Ingestion may cause nausea, vomiting, gastrointestinal irritation, headaches, blurred vision, dizziness and lowering of blood pressure. Repeated exposure of the eyes to high concentrations may cause reversible eye damage. Prolonged or repeated exposure may cause dermatitis. Chronic effects of overexposure may include kidney and/or liver damage and blood effects. Xylenes may be narcotic at high concentrations. Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. [32],[56],[51],[107],[55],[101]

**Toxicity: Moderate.**

TWA: 100 ppm (435 mg/m<sup>3</sup>) [1]

STEL: 150 ppm (655 mg/m<sup>3</sup>) [1]

CL: 200 ppm (870 mg/m<sup>3</sup>) averaged over 10 min period [56]

IDLH: 10000 ppm (43.5 g/m<sup>3</sup>) [56],[107]

Peak: 300 ppm (1300 mg/m<sup>3</sup>) for 30 min duration [107]

Odor threshold: 0.3-20 ppm (1.3-87 mg/m<sup>3</sup>) [104]

0.05 ppm (0.2 mg/m<sup>3</sup>) [107]

Carcinogenicity: negative in small animals with mixed xelenes [25],[26]

Mutagenicity: not mutagenic [101]

**Exposure:**

**External:**

Non-lethal: 200 ppm -- high to moderate irritation effects [51]

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: 50-500 mg/kg body wt. -- 50% chance of death [107]

**Inhalation:**

Short-term Inhalation Limits: 300 ppm (1300 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: 100 ppm (435 mg/m<sup>3</sup>) for 60 min -- unsatisfactory [104]

300 ppm (1300 mg/m<sup>3</sup>) for 60 min -- symptoms of illness [104]

1000 ppm (43.5 g/m<sup>3</sup>) for 60 min -- severe toxic effects [104]

Lethal: 6125 ppm (26.6 g/m<sup>3</sup>) for 12 hr [55]



p-Xylene

 $C_8H_{10}$ 

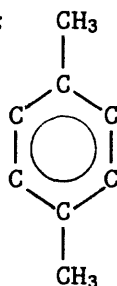
CAS RN: 106-42-3

Syn: p-Xylene \* Benzene, 1,4-dimethyl- \* Chromar \* 1,4-Dimethylbenzene \*  
 p-Dimethylbenzene \* p-Methyltoluene \* Scintillar \* UN 1307 (DOT) \* 1,4-  
 Xylene \* 4-Xylene \* para-Xylene \* p-Xylol \*

Molecular formula:  $p-C_6H_4(CH_3)_2$ 

Monocyclic Aromatic Hydrocarbon

Structural formula:



## Physical properties:

Relative molecular mass:	106.167	
Specific gravity:	0.8611	[10], [106], [22], [51], [105]
	0.86105	[14]
	0.86104	[108]
	0.861	[47], [107], [48]
	0.86	[32], [104]
Boiling point:	138.5°C	[47], [22]
	138.4°C	[104], [10]
	138.359°C	[49]
	138.35°C	[105]
	138.3°C	[32], [106], [107]
	137.°-138°C	[108]
Melting point:	13.3°C	[106], [10], [107], [48]
	13.263°C	[14], [49]
	13.26°C	[105]
	13.2°C	[47], [22]
	13.°C	[32], [104]
	13.°-14°C	[108]
Refractive index:	1.49582	[49]
	1.49581	[14]
	1.4958	[106], [10], [105]
	1.49575	[108]
Vapor pressure:	0.133 kPa @ -8.1°C (1mm)	[47], [105]
	0.666 @ 5°C (5mm)	[47]
	0.866 @ 20°C (6.5mm)	[104]
	1.20 @ 20°C (9mm)	[32]
	1.2 @ 25°C (9mm)	[49]
	1.333 @ 27.3°C (10mm)	[105], [51]
	1.600 @ 30°C (12mm)	[104]
Vapor density:	3.7	[32], [104]
	3.66	[51]
Evaporation rate:	0.7	[32]
Relative dielectric permittivity:	2.27 @ 20°C	[10], [105]
	2.2699 @ 20°C	[49]
	2.237 @ 25°C	[14]
Loss tangent:	unknown	

498 - *p*-Xylene

Relaxation time:	unknown		
Thermal conductivity:	unknown		
Electrical resistivity:	1.3x10 <sup>7</sup> MOhm-m		[49]
	>1.0x10 <sup>7</sup>		[10]
Critical temperature:	345.0°C		[105], [48]
	343.08°C		[49]
	343.0°C		[10], [107]
Critical pressure:	3.511 MPa		[10], [49]
	3.510		[107]
	3.435		[105]
Dynamic viscosity:	0.696 mPa-s @ 16°C		[105]
	0.648 @ 20°C		[105]
	0.644 @ 20°C	[14], [10], [49]	
	0.605 @ 25°C		[49]
	0.566 @ 30°C		[49]
	0.513 @ 40°C		[105]
Kinematic viscosity:	0.808 μm <sup>2</sup> /s @ 16°C		
	0.753 @ 20°C		
	0.748 @ 20°C		
	0.703 @ 25°C		
	0.657 @ 30°C		
	0.596 @ 40°C		
Surface tension:	29.079 mN/m @ 15°C		[10]
([10] values are calculated)	28.3 @ 20°C		[107]
	28.31 @ 20°C	[14], [49]	
	28.37 @ 20°C		[105]
	28.542 @ 20°C		[10]
	27.76 @ 25°C		[49]
	27.22 @ 30°C		[14]
	27.468 @ 30°C		[10]
	26.13 @ 40°C		[14]
	26.394 @ 40°C		[10]
	25.320 @ 50°C		[10]
	24.246 @ 60°C		[10]
	23.172 @ 70°C		[10]
	22.098 @ 80°C		[10]
	21.024 @ 90°C		[10]
	19.950 @ 100°C		[10]
Contact angle: [18]			
	sessile	advancing	receding
quartz	5	7	0
calcite	6	7	17
biotite	11	10	0
Ca-mont.	5	7	0
Thermal expansion coefficient:	0.000956 K <sup>-1</sup>		[49]
	0.00102 K <sup>-1</sup> @ 20°C		[48]
Compressibility:	0.8588 nPa <sup>-1</sup> @ 25°C		[49]
Vapor diffusivity:	6.7 μm <sup>2</sup> /s @ 25°C		[59]
Solution diffusivity:	0.71 nm <sup>2</sup> /s (calc)		[59]
Electric dipole moment:	0.		[10], [105]
	0.0667x10 <sup>-30</sup> C-m @ 20°-60°C (liq)		[49]
Ionization potential:	8.44 eV (PI)		[105]
Magnetic volume susceptibility:	-7.824x10 <sup>-6</sup> SI units @ 20°C		[105]

Speed of sound:	unknown		
Heat of melting:	17.113 kJ/mol		[49]
	17.1		[10], [14]
	16.81		[107]
	16.805		[105]
Heat of vaporization:	36.1 kJ/mol		[107]
	36.0		[10]
	35.98 @ bp		[49]
	42.376 @ 25°C		[49]
	41.0421		[105]
	42.41 @ 25°C		[14]
Heat of sublimation:	42.41 kJ/mol		[10]
Heat capacity @ 25°C:	0.1825 kJ/(mol-K) (liq)		[105]
	0.18166 (liq)		[49]
	0.1269 (gas)	[10],	[105]
Heat of combustion:	-4555.91 kJ/mol @ 25°C (liq)		[20]
	-4552.86 (liq)		[49]
	-4598.32 (gas)		[20]
	-4559.8 @ 20°C (liq)		[105]
Heat of formation:	-24.45 kJ/mol @ 25°C (liq)		[10]
	-24.426 (liq)		[49]
	-24.37 (liq)		[20]
	18.00 (gas)	[49],	[20]
	17.96 (gas)		[10]
Gibbs (free) energy:	110.15 kJ/mol @ 25°C (liq)		[10]
	121.21 (gas)		[10]
Analytical chemistry:	pP <sub>oct</sub> = 3.15	[104], [21], [101], [59],	[24]
	pK <sub>s</sub> unknown		
	pK <sub>a</sub> >15.		[59]
	pK <sub>BH</sub> = 5.7 @ 0°C in HF		[49]
Henry's law constant =	0.778 kPa-m <sup>3</sup> /mol		[24]
	0.72		[41]
	0.64 @25°C		[41]
	0.314 dimensionless (calc)		[59]
Hydrolysis half-life = unknown			

**Electrochemical data:** Neikam and Desmond (1964), Meites and Zuman (1977), Nyberg (1978), Anderson and Stocker (1983), Ebersson and Utley (1983b)

**Clay-organic interaction data:** Xylene increases the hydraulic conductivity of clay soils (Anderson and Brown, 1981; Anderson and Jones, 1983; Anderson et al., 1981; Brown and Thomas, 1984; Brown et al., 1986; Lord et al., 1983; Rao et al., 1988; Schramm et al., 1986). Physical adsorption of xylenes and coordination to the exchangeable cations when intercalated by Cu(II)montmorillonite. Frequencies of C-C stretching and C-H out-of-plane vibrations of p-xylene in the liquid state and when adsorbed by Cu(II)montmorillonite. (Theng, 1974). Also see Pinnavaia and Mortland (1971)

## 500 - *p*-Xylene

**Solubility:** Almost insoluble in water. Miscible with ethanol, ether, acetone, carbon tetrachloride, petroleum ether, benzene and many other organic solvents. [108],[51],[32],[49],[104]

0.00003 wt% in water @ 20°C [32]

0.0156 wt% in water @ 25°C [49]

0.0198 wt% in water @ 25°C [104]

**Form:** Clear, colorless liquid (plates or prisms at low temperatures). Characteristic aromatic benzene-like odor. [32],[104],[108],[51],[107]

**Use:** Intermediate during the manufacture of plastics, synthetics and mixed/pure isomers; diluter or solvent in surface coatings, printing operations and manufacture of rubber; degreasing agent in plastics and electronics; solvent for alkyd resins, lacquers, enamels, rubber cements; in organic synthesis reactions and manufacture of epoxy resins; in formulation of insecticides; in manufacture of xylene-formaldehyde resins, pharmaceuticals, vitamins, leather, dyes and other organics; sterilizing agent for catgut; with Canadian balsam as oil-immersion in microscopy; cleaning agent in microscope techniques; raw material for production of benzoic acid, phthalic anhydride, isophthalic and terephthalic acids as well as their dimethyl esters used in the manufacture of polyester fibers ("Dacron", "Mylar", "Terylene"); aviation gasolines; 6.8 wt% in high octane number gasoline. [32],[104],[108],[56]

**Fire and explosion hazard:** High.

Flash point: (CC) 27.2°C [107],[22],[32]

(OC) 23°C [14]

(OC) 25°C [51]

UEL: 7.0% [51],[32],[14]

6.6% [107]

LEL: 1.1% [107],[51],[32],[14]

Autoign. temp.: 530°C [51],[32]

465°C [107]

Highly flammable liquid. Dangerous fire hazard when exposed to heat or flame. Flashback along vapor trail may occur. Moderate explosion hazard in the form of vapor when exposed to heat or flame. Vapor may explode if ignited in an enclosed area. When heated to decomposition it emits acrid smoke and toxic fumes or vapors (CO, CO<sub>2</sub>). Contact with strong oxidizers may cause fires and explosions. Fight fire with CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. Water may be ineffective. [51],[107],[55]

**Incompatibility:** Strong oxidizers; acetic acid + air; HNO<sub>3</sub>; 1,3-dichloro-5,5-dimethyl-2,4-imid-axolidindione. [51]

**Handling:** Keep away from heat, sparks and flame. Avoid breathing vapors (appropriate respirator or self-contained breathing apparatus). Avoid contact with eyes, skin or clothing (nitrile or PVA synthetic latex gloves and boots; safety goggles or face shield; lab coat, apron). Use with adequate ventilation (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Bond and ground containers when transferring liquid. Store in cool, dry, well-ventilated, flammable liquid storage area. [56],[57],[53],[32]

**Health effects:** Xylenes are moderately toxic. Routes of entry are inhalation of vapor slight percutaneous absorption of liquid, ingestion, and skin and eye contact. Points of attack include central nervous system, eyes, gastrointestinal tract, blood, liver, kidneys, and skin. Vapor may cause irritation of the eyes, nose and throat. At high concentration, it may cause severe breathing difficulties (effects may be delayed), dizziness, staggering, drowsiness and unconsciousness. Also, breathing high concentrations may cause loss of appetite, nausea, vomiting and abdominal pain. Ingestion may cause nausea, vomiting, gastrointestinal irritation, headaches, blurred vision, dizziness and lowering of blood pressure. Repeated exposure of the eyes to high concentrations may cause reversible eye damage. Prolonged or repeated exposure may cause dermatitis. Chronic effects of overexposure may include kidney and/or liver damage. Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. Xylenes may be narcotic at high concentrations. [32],[56],[51],[107],[55],[101]

**Toxicity:** Moderate.

TWA: 100 ppm (435 mg/m<sup>3</sup>) [1]

STEL: 150 ppm (665 mg/m<sup>3</sup>) [1]

CL: 200 ppm (870 mg/m<sup>3</sup>) averaged over 10 min period [56],[51]

IDLH: 10000 ppm (43.5 g/m<sup>3</sup>) [56]

Peak: 300 ppm (1300 mg/m<sup>3</sup>) for 30 min duration [107]

Odor threshold: 200 ppm (870 mg/m<sup>3</sup>) -- rapid olfactory fatigue [32]

0.05 ppm (0.2 mg/m<sup>3</sup>) [107]

0.5-8 ppm (2-35 mg/m<sup>3</sup>) -- detection [104]

2 ppm (8.7 mg/m<sup>3</sup>) -- recognition [104]

Carcinogenicity: negative in small animals with mixed xelenes [25],[26]

Mutagenicity: unknown

**Exposure:**

**External:**

Non-lethal: 200 ppm (870 mg/m<sup>3</sup>) -- eye irritation, anorexia, nausea, vomiting, and abdominal pain [32]

Lethal: unknown

**Oral:**

Non-lethal: unknown

Lethal: 50-500 mg/kg body wt. -- 50% chance of death [107]

**Inhalation:**

Short-term Inhalation Limits: 300 ppm (1300 mg/m<sup>3</sup>) for 30 min [107]

Non-lethal: unknown

Lethal: unknown

## 502 - 2,4-Xylenol

2,4-Xylenol

C<sub>8</sub>H<sub>10</sub>O

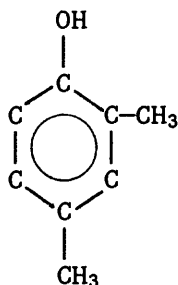
CAS RN: 105-67-9

Syn: 2,4-Xylenol \* Phenol, 2,4-dimethyl- \* 2,4-Dimethylphenol \* 4,6-Dimethylphenol \* 2,4-DMP \* 1-Hydroxy-2,4-dimethylbenzene \* 4-Hydroxy-1,3-dimethylbenzene \* RCRA Waste Number U101 \* UN 2261 (DOT) \* 1,3,4 Xylenol \* m-Xylenol \* (as)(m)-Xylenol \*

Molecular formula: 2,4-(CH<sub>3</sub>)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>-OH

Monohydric Phenol

Structural formula:



## Physical properties:

Relative molecular mass:	122.167	
Specific gravity:	1.036	[104]
	0.9650	[105]
Boiling point:	211.5°C	[104]
	210.931°C	[49]
	210.°C	[106], [105]
Melting point:	27.°-28.°C	[105]
	27.°C	[10], [14], [106]
	26.°C	[104]
	25.4°-26°C	[23]
	24.54°C (fp)	[49]
Refractive index:	1.5390 @ 20°C	[10]
	1.5420 @ 14°C	[105]
	1.5424 @ 50°C	[49]
Vapor pressure:	0.013 kPa @ 25°C (0.098mm)	[23]
	0.02178 @ 25°C (0.16mm)	[14], [49]
	0.133 @ 51.8°C (1mm)	[105]
	1.33 @ 92.3°C (10mm)	[105]
Vapor density:	unknown	
Evaporation rate:	unknown	
Relative dielectric permittivity:	6.61 @ 30°C	[49]
Loss tangent:	unknown	
Relaxation time:	unknown	
Thermal conductivity:	unknown	
Electrical resistivity:	unknown	
Critical temperature:	434.4°C	[49], [10]
Critical pressure:	4.357 MPa	[10]
	6.6	[49]
Dynamic viscosity:	unknown	
Kinematic viscosity:	unknown	
Surface tension:	0.03123 mN/m @ 40°C	[49]
Contact angle:	unknown	
Thermal expansion coefficient:	0.000818 K <sup>-1</sup>	[49]
Compressibility:	unknown	
Vapor diffusivity:	unknown	

Solution diffusivity:	unknown	
Electric dipole moment:	$5.67 \times 10^{-30}$ C-m @ 20°C (liq)	[49]
Ionization potential:	unknown	
Magnetic volume susceptibility:	unknown	
Speed of sound:	unknown	
Heat of melting:	unknown	
Heat of vaporization:	54.9735 kJ/mol	[105]
	65.856 @ 25°C	[49]
	47.145 @ bp	[49]
Heat of sublimation:	65.90 kJ/mol	[10]
Heat capacity @ 25°C:	unknown	
Heat of combustion:	-4348.47 kJ/mol @ 25°C (liq)	[49]
Heat of formation:	-228.82 kJ/mol @ 25°C (liq)	[49]
	-162.97 (gas)	[49]
	-163.0 (gas)	[10]
Gibbs (free) energy:	unknown	
Analytical chemistry: $pP_{oct}$ =	2.5	[8], [41]
	2.42	[27], [41]
	2.30	[23], [21]
$pK_s$ =	unknown	
$pK_a$ =	10.58	[10]
	10.60	[8]
	10.63	[49], [23]
$pK_{BH}$ =	unknown	
Henry's law constant =	0.000664 kPa-m <sup>3</sup> /mol (est)	[41]
Hydrolysis half-life =	NA	[8]

Electrochemical data: Meites and Zuman (1977)

Clay-organic interaction data: Unknown

Solubility: Slightly soluble in water. Miscible with ethanol, ether, alkali, chloroform, and benzene. [105], [49]

0.42 wt% in water @ 20°C	[41]
0.787 wt% in water @ 25°C	[49]
0.62 wt% in water @ 25°C	[23]

Form: Colorless needles or liquid. [104]

Use: Manufacture of phenolic antioxidants, pharmaceuticals, plastics and resins, solvents, disinfectants (microbicide), insecticides and fungicides, rubber chemicals, polyphenylene oxide, wetting agents, dyestuffs; coal processing; coal tar fractionation; constituent in cresylic acid; gasoline additive. Coal is a natural source. [104], [41]

## 504 - 2,4-Xylenol

**Fire and explosion hazard:** Low

Flash point: >110°C [41]

UEL: unknown

LEL: unknown

Autoign. temp.: unknown

Slightly flammable liquid or solid. Emits acrid smoke and fumes, including CO and CO<sub>2</sub>, when heated to decomposition. Material may decompose to form flammable and/or explosive mixtures in air. Fight fire with water spray, CO<sub>2</sub>, dry chemical powder, alcohol or polymer foam. [107],[55]

**Incompatibility:** Bases; acid chlorides; acid anhydrides; oxidizing agents; corrodes steel; brass; copper, copper alloys. [55]

**Handling:** Avoid heat, sparks, flame, and sources of ignition. Do not breathe dust or mist (appropriate respirator or self-contained breathing apparatus required). Do not get in eyes, on skin, or on clothing (resistant gloves, safety goggles or faceshield (8-inch minimum), other protective clothing). Readily absorbed through skin. Avoid prolonged or repeated exposure. Safety shower and eye bath should be provided. It is corrosive. Keep container tightly closed. Store in a cool, dry, secure poison area suitable for corrosives. [55]

**Health effects:** 2,4-Xylenol is a strong irritant. Routes of entry are inhalation, ingestion, skin absorption, and eye and skin contact. Points of attack include eyes, skin, and respiratory system. Contact causes burns. It is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes and skin. Inhalation may be fatal as a result of spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis and pulmonary edema. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea and vomiting. [55]

**Toxicity:** Low

TWA: no value set [1]

STEL: no value set [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: 0.0002 ppm (0.001 mg/m<sup>3</sup>) -- recognition [104]

0.0001-0.08 ppm (0.0005-0.4 mg/m<sup>3</sup>) -- detection [104]

Carcinogenicity: unknown

Mutagenicity: unknown

**Exposure:** Unknown



Zinc

Zn

CAS RN: 7440-66-6

Syn: Zinc \* Zn \* Asarco L 15 \* Blue powder \* C.I. 77945 \* C.I. Pigment black 16 \* C.I. Pigment metal 6 \* Emanay zinc dust \* Granular zinc \* Jasad \* Merrillite \* Non-pyrophoric zinc \* Pasco \* Pyrophoric zinc \* UN 1383 (DOT) \* UN 1436 (DOT) \* Zinc dust \* Zinc powder \*

Molecular formula: Zn

Element

**Physical properties:**

Relative molecular mass:	65.38	[105]
Specific gravity:	7.14	[22],[47],[51],[108],[105]
Boiling point:	911.°C	[10]
	908.°C	[51],[108]
	907.°C	[22],[47],[105]
Melting point:	419.8°C	[51]
	419.6°C	[10]
	419.58°C	[105]
	419.5°C	[108]
	419.4°C	[47]
Refractive index:	NA	
Vapor pressure:	0.133 kPa @ 487°C (1mm)	[47],[51]
Vapor density:	2.2	[55]
Evaporation rate:	NA	
Relative dielectric permittivity:	NA	
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	119. W/(m-K) @ 0°C	[20]
	116. @ 25°C	[105]
Electrical resistivity:	5.479x10 <sup>-14</sup> MOhm-m @ 0°C	[105]
	5.964x10 <sup>-14</sup> @ 20°C	[105]
	6.x10 <sup>-14</sup> @ 22°C	[105]
Critical temperature:	unknown	
Critical pressure:	unknown	
Dynamic viscosity:	1.68 mPa-s @ 280°C	[105]
Kinematic viscosity:	0.235 µm <sup>2</sup> /s @ 280°C	[105]
Surface tension:	761. mN/m @ 419.5°C	[105]
	753. @ 477°C	[20]
	708. @ 590°C	[20]
Contact angle:	NA	
Thermal expansion coefficient:	0.029 K <sup>-1</sup>	[48]
Compressibility:	NA	
Vapor diffusivity:	unknown	
Solution diffusivity:	unknown	
Electric dipole moment:	NA	
Ionization potential:	9.391 eV (S)	[105]
Magnetic volume susceptibility:	-143.2x10 <sup>-6</sup> SI units	[105]
Speed of sound:	4210. m/s	[105]
Heat of melting:	7.390 kJ/mol	[10]
	6.678	[105]
Heat of vaporization:	115.64 kJ/mol	[10]
Heat of sublimation:	unknown	

## 506 - Zinc

Heat capacity @ 25°C:	0.0254 kJ/(mol-K)	(sol)	[10]
	0.0252	(sol)	[105]
	0.0208	(gas)	[10]
Heat of combustion:	unknown		
Heat of formation:	0.00 kJ/mol @ 25°C	(sol)	[10],[47]
	-152.5	(liq)	[105]
	130.82	(gas)	[10]
	130.6	(gas)	[105]
Gibbs (free) energy:	0.00 kJ/mol @ 25°C	(sol)	[47]
	-147.31	(liq)	[105]
	95.24	(gas)	[10]
	95.00	(gas)	[105]

Analytical chemistry:  $pP_{oct}$  - NA  
 $pK_s$  - NA  
 $pK_a$  - NA  
 $pK_{BH}$  - NA  
Henry's law constant - NA  
Hydrolysis half-life - NA

Electrochemical data: Brodd and Leger (1976)

Clay-organic interaction data: inorganic

**Solubility:** Insoluble in water. Soluble in acids and alkalies. Slowly attacked by  $H_2SO_4$  or  $HCl$ . Oxidizing agents or metal ions ( $Cu^{2+}$ ,  $Ni^{2+}$ ,  $Co^{2+}$ ) accelerate the process. [22],[47],[108]

**Form:** Zinc is a bluish-white, lustrous metal, brittle at ordinary temperatures but malleable at 100° to 150°C and brittle and pulverizable at 210°C, with distorted hexagonal close-packed structure. It has atomic number 30 (Group IIB) and valence of 2. Commercially available forms are ingots, lumps, sheets, wire, shot, strips, sticks, granules, mossy, and dust or powder. It is stable in dry air and becomes covered with a white coating of basic carbonate on exposure to moist air. Zinc is not found in its native state. Principal ores are sphalerite, smithsonite, calamine, and franklinite. [22],[51],[108],[105]

**Use:** In galvanizing sheet iron; as an ingredient of alloys such as bronze, brass, Babbitt metal, German silver, and special alloys for die-casting; as a protective coating for other metals to prevent corrosion; for electrical apparatus, especially dry cell batteries, household utensils, castings, printing plates, building materials, railroad car linings, automotive equipment; as reducing agent in organic chemistry; for deoxidizing bronze; extracting gold by the cyanide process, purifying fats for soaps; bleaching bone glue; manufacture sodium hydrosulfite; insulin zinc salts; as reagent in analytical chemistry, e.g., in the Marsh and Gutzeit test for arsenic; as a reducer in the determination of iron. It is a nutritional trace element. [108],[105]

**Fire and explosion hazard:** Low

Flash point: unknown

UEL: unknown

LEL: unknown

Autoign. temp.: unknown

Flammable solid. Moderate fire hazard in the form of dust when exposed to heat or flame. Moderate explosion hazard in the form of dust when reacted with acids. The presence of moisture can result in spontaneous combustion. Burns in air with a bluish-green flame. Fight fire with special mixtures of dry chemical (class D fire extinguishing material only). [22],[51],[55]

**Incompatibility:** Acids; strong alkalis; chlorides; chlorates; chlorinated solvents; amines; oxides, nitrates; fluorine; carbon disulfide;  $\text{NH}_4\text{NO}_3$ ;  $\text{BaO}_2$ ;  $\text{Ba}(\text{NO}_3)_2$ ; cadmium;  $\text{Cl}_2$ ;  $\text{ClF}_3$ ;  $\text{CrO}_3$ ; (ethyl acetoacetate + tribromoneopentyl alcohol); hydrazine mononitrate; hydroxylamine;  $\text{Pb}(\text{N}_3)_2$ ;  $(\text{Mg} + \text{Ba}(\text{NO}_3)_2 + \text{BaO}_2)$ ;  $\text{MnCl}_2$ ;  $\text{HNO}_3$ ; performic acid;  $\text{KClO}_3$ ;  $\text{KNO}_3$ ;  $\text{K}_2\text{O}_2$ ; selenium;  $\text{NaClO}_3$ ;  $\text{Na}_2\text{O}_2$ ; sulfur; tellurium;  $\text{H}_2\text{O}$ ;  $(\text{NH}_4)_2\text{S}$ ;  $\text{As}_2\text{O}_3$ ;  $\text{CS}_2$ ;  $\text{CaCl}_2$ ;  $\text{NaOH}$ ; chlorinated rubber; catalytic metals; halocarbons; o-nitroanisole; nitrobenzene; non-metals; oxidants; paint primer base; pentacarbonyliron; transition metal halides; seleninyl bromide. [51],[108],[55]

**Handling:** Keep away from heat and open flame when in the form of dust or powder. Do not breathe vapor, dust or powder (appropriate respirator or self-contained breathing apparatus). Do not get in eyes, on skin, or on clothing (chemical resistant gloves and suit; safety goggles or face shield). Immediately remove contaminated clothing. Immediately wash if skin is wet or contaminated. Use only in well-ventilated area (fume hood). Safety shower and eye bath stations should be provided. Keep container tightly closed. Store in a cool, dry area. Air and moisture sensitive. [55],[56],[57]

**Health effects:** Zinc is not inherently a toxic element but can be an irritant. Routes of entry are inhalation of dust and fumes, ingestion of soluble salts, skin absorption, and eye and skin contact. Points of attack include respiratory system, lungs, skin, eyes. Pure zinc powder, dust and fume is relatively non-toxic to humans. Problems arise from oxidation of zinc fumes before inhalation or the presence of impurities such as Cd, Sb, As, and Pb. Inhalation of fumes may result in sweet taste, throat dryness, cough, weakness, generalized aching, chills, fever, nausea, vomiting. Overexposure can cause lung irritation, chest pain and edema which may be fatal. Zinc chloride fumes have caused injury to mucous membranes and skin and eye irritation. Ingestion of soluble salts may cause nausea, vomiting, purging. [108],[56],[51],[55],[102]

**Toxicity:** Low

TWA: no value set for zinc metal [1]

STEL: no value set for zinc metal [1]

CL: unknown

IDLH: unknown

Peak: unknown

Odor threshold: unknown

Carcinogenicity: unknown

Mutagenicity: unknown

508 - Zinc

Exposure:

External:

Non-lethal: 300  $\mu$ g for 3 days intermittent -- mild skin irritation [51]

Lethal: unknown

Oral: unknown

Inhalation:

Short-term Inhalation Limits: unknown

Non-lethal: 46 ppm (124 mg/m<sup>3</sup>)/50 min -- pulmonary system effects [51]

Lethal: unknown

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## INDEX OF SYNONYMS

Synonyms for the substances found in this report are listed in alphabetical sequence on the following pages. Substances as they appear in the Contents are included with page numbers. The many prefixes used in organic chemistry (such as *ortho-*, *meta-*, *para-*, *o-*, *m-*, *p-*, *alpha-*, *beta-*, *gamma-*, *delta-*, *sym-*, *asym-*, *unsym-*, *trans-*, *N-*,  $\alpha$ ,  $\beta$ ,  $\gamma$ ) and numerals which denote structure are ignored in alphabetizing because they are not considered an integral part of the name. However, other prefixes (such as *bis*, *di-*, and *tri-*) are considered an important part of the name and are placed in normal alphabetical order. Upper and lower case letters were treated the same. Commas and hyphens were ignored.

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- Aadibroom. See 1,2-Dibromoethane.  
 Aahepta. See Heptachlor.  
 Aalindan. See  $\gamma$ -Hexachlorocyclohexane.  
 Aavero-extra. See DDT.  
 Absolute Ethanol. See Ethanol.  
 Acetic acid. page 85.  
 Acetone. page 90.  
 trans-Acetylene dichloride. See trans-1,2-Dichloroethene.  
 Acetylene tetrachloride. See 1,1,2,2-Tetrachloroethane.  
 Acetylene trichloride. See Trichloroethene.  
 Acquinite. See Acrolein.  
 Acraldehyde. See Acrolein.  
 Acritet. See Acrylonitrile.  
 Acrolein. page 96.  
 Acrolein, inhibited. See Acrolein.  
 trans-Acrolein. See Acrolein.  
 Acrylaldehyde. See Acrolein.  
 Acrylic aldehyde. See Acrolein.  
 Acrylon. See Acrylonitrile.  
 Acrylonitrile. page 100.  
 Acrylonitrile, inhibited. See Acrylonitrile.  
 Acrylonitrile monomer. See Acrylonitrile.  
 Acutox. See Pentachlorophenol.  
 Aerothane. See 1,1,1-Trichloroethane.  
 Aerothene. See 1,1,1-Trichloroethane.  
 Aerothene MM. See Dichloromethane.  
 Aerothene TT. See 1,1,1-Trichloroethane.  
 Aethylis. See Chloroethane.  
 Aethylis chloridum. See Chloroethane.  
 Aficide. See  $\gamma$ -Hexachlorocyclohexane.  
 Ag. See Silver.  
 Agricide maggot killer (F). See Toxaphene.  
 Agrisol G-20. See  $\gamma$ -Hexachlorocyclohexane.  
 Agritan. See DDT.  
 Agroceres. See Heptachlor.  
 Agrocide (2, 7, 6G, III, or WP). See  $\gamma$ -Hexachlorocyclohexane.  
 Agronexit. See  $\gamma$ -Hexachlorocyclohexane.  
 Albocarbon. See Naphthalene.  
 Alcohol. See Ethanol.  
 Aldifen. See 2,4-Dinitrophenol.  
 Aldocit. See Aldrin.  
 Aldrec. See Aldrin.  
 Aldrex. See Aldrin.  
 Aldrex 30. See Aldrin.  
 Aldrin. page 104.  
 Aldrin epoxide. See Dieldrin.  
 Aldrite. See Aldrin.  
 Aldrosol. See Aldrin.  
 Algofrene type 1. See Trichlorofluoromethane.  
 Algofrene type 2. See Dichlorodifluoromethane.  
 Algrain. See Ethanol.  
 Algylen. See Trichloroethene.  
 Allbri natural copper. See Copper.  
 Alltex. See Toxaphene.  
 Alltox. See Toxaphene.  
 Allyl aldehyde. See Acrolein.  
 Alvit. See Dieldrin.  
 Alvit 55. See Dieldrin.  
 Am-fol. See Ammonia.  
 Amatin. See Hexachlorobenzene.  
 Ameisenmittel merck. See  $\gamma$ -Hexachlorocyclohexane.  
 Ameisentod. See  $\gamma$ -Hexachlorocyclohexane.  
 Aminobenzene. See Aniline.  
 Aminophen. See Aniline.  
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 Ammonia gas. See Ammonia.  
 AN. See Acrylonitrile.  
 Anac 110. See Copper.  
 Anamenth. See Trichloroethene.  
 Anatox. See Toxaphene.  
 Anhydrol. See Ethanol.  
 Anhydrous alcohol. See Ethanol.  
 Anhydrous ammonia. See Ammonia.  
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 Aniline oil. See Aniline.  
 Ankilostin. See Tetrachloroethene.  
 (6)Annulene. See Benzene.  
 Anodynnon. See Chloroethane.  
 Anofex. See DDT.  
 Anozol. See Diethyl phthalate.  
 Anprolene. See Ethylene oxide.  
 Anticarie. See Hexachlorobenzene.  
 Antisal 1A. See Toluene.  
 Antisol 1. See Tetrachloroethene.  
 Anyvim. See Aniline.  
 Aparasin. See  $\gamma$ -Hexachlorocyclohexane.  
 Aphitiria. See  $\gamma$ -Hexachlorocyclohexane.  
 Aplidal. See  $\gamma$ -Hexachlorocyclohexane.  
 Aptal. See 6-Chloro-m-cresol.  
 Aqualin. See Acrolein.  
 Aqualine. See Acrolein.  
 Arbitex. See  $\gamma$ -Hexachlorocyclohexane.  
 Arcton 6. See Dichlorodifluoromethane.  
 Arcton 9. See Trichlorofluoromethane.  
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 Arsenic black. See Arsenic.  
 Arsenicals. See Arsenic.  
 Artic. See Chloromethane.  
 Arwood copper. See Copper.  
 Arylamine. See Aniline.

- Asarco L 15. See Zinc.
- Asordin. See Carbon tetrachloride.
- Asymmetrical dichloroethane. See 1,1-Dichloroethane.
- Attac 4-2. See Toxaphene.
- Attac 4-4. See Toxaphene.
- Attac 6. See Toxaphene.
- Attac 6-3. See Toxaphene.
- Attac 8. See Toxaphene.
- Avlothane. See Hexachloroethane.
- Avolin. See Dimethyl phthalate.
- 1-Azanaphthalene. See Quinoline.
- Azotox M-33. See DDT.
- B-500. See Quinoline.
- BA. See Benz[a]anthracene.
- B(a)A. See Benz[a]anthracene.
- Baker's P and S liquid and ointment. See Phenol.
- Baktol. See 6-Chloro-m-cresol.
- Baktolan. See 6-Chloro-m-cresol.
- Baltana. See 1,1,1-Trichloroethane.
- Basaklor. See Heptachlor.
- BbF. See Benz(e)acephenanthrylene.
- BbFL. See Benz(e)acephenanthrylene.
- BBH. See  $\gamma$ -Hexachlorocyclohexane.
- BCEE. See Bis(2-chloroethyl) ether.
- BCME. See Bis(chloromethyl) ether.
- Be. See Beryllium.
- BEHP. See Bis(2-ethylhexyl) phthalate.
- Belt. See Chlordane.
- Ben-hex. See  $\gamma$ -Hexachlorocyclohexane.
- Bentox 10. See  $\gamma$ -Hexachlorocyclohexane.
- Benxol. See  $\gamma$ -Hexachlorocyclohexane.
- 1,2-Benzacenaphthene. See Fluoranthene.
- Benz(e)acephenanthrylene. page 124.
- 3,4-Benz(e)acephenanthrylene. See Benz(e)acephenanthrylene.
- 1-Benzanine. See Quinoline.
- Benzanthracene. See Benz[a]anthracene.
- Benz[a]anthracene. page 127.
- 1,2-Benzanthracene. See Benz[a]anthracene.
- 1,2-Benz(a)anthracene. See Benz[a]anthracene.
- 1,2:5,6-Benzanthracene. See Dibenz[a,h]anthracene.
- Benzanthrene. See Benz[a]anthracene.
- 1,2-Benzanthrene. See Benz[a]anthracene.
- 1-Benzazine. See Quinoline.
- Benzenamine. See Aniline.
- Benzenamine, N-nitroso-N-phenyl-. See N-Nitrosodiphenylamine.
- Benzene. page 130.
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- Benzene hexachloride. See  $\gamma$ -Hexachlorocyclohexane.
- Benzene hexachloride-gamma isomer. See  $\gamma$ -Hexachlorocyclohexane.
- $\gamma$ -Benzene hexachloride. See  $\gamma$ -Hexachlorocyclohexane.
- Benzene hexahydride. See Cyclohexane.
- Benzene, amino. See Aniline.
- Benzene, chloro-. See Chlorobenzene.
- Benzene, 1,2-dichloro-. See 1,2-Dichlorobenzene.
- Benzene, 1,3-dichloro-. See 1,3-Dichlorobenzene.
- Benzene, 1,4-dichloro-. See 1,4-Dichlorobenzene.
- Benzene, 1,2-dimethyl-. See o-Xylene.
- Benzene, 1,3-dimethyl-. See m-Xylene.
- Benzene, 1,4-dimethyl-. See p-Xylene.
- Benzene, ethyl. See Ethylbenzene.
- Benzene, hexachloro-. See Hexachlorobenzene.
- Benzene, methyl-. See Toluene.
- Benzene, 1-methyl-2,4-dinitro-. See 2,4-Dinitrotoluene.
- Benzene, 2-methyl-1,3-dinitro-. See 2,6-Dinitrotoluene.
- Benzene, nitro-. See Nitrobenzene.
- Benzene, 1,2,4-trichloro-. See 1,2,4-Trichlorobenzene.
- Benzene, 1,1'-(2,2,2-trichloro-ethylidene)bis[4-chloro-. See DDT.
- Benzenecarboxylic acid. See Benzoic acid.
- o-Benzenedicarboxylic acid dibutyl ester. See Dibutyl phthalate.
- Benzene-o-dicarboxylic acid di-n-butyl ester. See Dibutyl phthalate.
- 1,2-Benzene-dicarboxylic acid, dibutyl ester. See Dibutyl phthalate.
- 1,2-Benzenedicarboxylic acid, diethyl ester. See Diethyl phthalate.
- 1,2-Benzenedicarboxylic acid, dimethyl ester. See Dimethyl phthalate.
- 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester. See Bis(2-ethylhexyl)phthalate.
- Benzeneformic acid. See Benzoic acid.
- Benzene-cis-hexachloride. See  $\gamma$ -Hexachlorocyclohexane.
- gamma-benzene hexachloride. See  $\gamma$ -Hexachlorocyclohexane.
- Benzenemethanoic acid. See Benzoic acid.
- Benzenol. See Phenol.
- 2,3-Benzfluoranthene. See Benz(e)acephenanthrylene.
- 3,4-Benzfluoranthene. See Benz(e)acephenanthrylene.
- Benzidam. See Aniline.
- Benzidine. page 136.
- Benzidine base. See Benzidine.
- 1-Benzine. See Quinoline.
- Benzinoform. See Carbon tetrachloride.
- Benzinol. See Trichloroethene.
- Benzoanthracene. See Benz[a]anthracene.
- Benzo(a)anthracene. See Benz[a]anthracene.

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 Benzoate. See Benzoic acid.  
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 Benzo(b)fluoranthene. See Benz(e)acephenanthrylene.  
 Benzo(e)fluoranthene. See Benz(e)acephenanthrylene.  
 2,3-Benzofluoranthene. See Benz(e)acephenanthrylene.  
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 2,3-Benzofluoranthrene. See Benz(e)acephenanthrylene.  
 Benzo(jk)fluorene. See Fluoranthene.  
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 Benzopyridine. See Quinoline.  
 Benz(a)phenanthrene. See Chrysene.  
 1,2-Benzphenanthrene. See Chrysene.  
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 Benz(a)pyrene. See Benzo[a]pyrene.  
 3,4-Benz(a)pyrene. See Benzo[a]pyrene.  
 1,2-Benzpyrene. See Benzo[a]pyrene.  
 3,4-Benzypyrene. See Benzo[a]pyrene.  
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 $\gamma$ -BHC. See  $\gamma$ -Hexachlorocyclohexane.  
 gamma-BHC. See  $\gamma$ -Hexachlorocyclohexane.  
 p,p'-Bianiline. See Benzidine.  
 P,P'-Bianiline. See Benzidine.  
 4,4'-Bianiline. See Benzidine.  
 Bicarburet of hydrogen. See Benzene.  
 1,2-Bichloridiethane. See 1,2-Dichloroethane.  
 1,2-bichloroethane. See 1,2-Dichloroethane.  
 Biocide. See Acrolein.  
 Biphenyl, 4,4'-diamino-. See Benzidine.  
 [1,1'-Biphenyl]-4,4'-diamine. See Benzidine.  
 4,4'-Biphenyldiamine. See Benzidine.  
 4,4'-Biphenylenediamine. See Benzidine.  
 Bis( $\beta$ -chloroethyl) ether. See Bis(2-chloroethyl) ether.  
 Bis(2-chloroethyl) ether. page 150.  
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 Bis(chloromethyl) ether. page 154.  
 $\alpha,\alpha$ -bis(p-chlorophenyl)- $\beta,\beta,\beta$ -trichloroethane. See DDT.  
 1,1'-bis(p-chlorophenyl)-2,2,2-trichloroethane. See DDT.  
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 3,4-BP. See Benzo[a]pyrene.  
 BP. See Benzo[a]pyrene.  
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 3-Butanone. See 2-Butanone.  
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