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PHYSICAL AND CHEMICAL PROPERTIES AND HEALTH EFFECTS OF THIRTY-THREE TOXIC ORGANIC CHEMICALS

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CONTENTS

	Page
Introduction	4
The Properties	6
Abbreviations	13
Conversion Factors	16
Summary Tables	17
Acetic acid	27
Acetone	31
Benzene	34
Bis(2-ethylhexyl)phthalate	37
Bromoform	39
Carbon tetrachloride	42
Chlorobenzene	46
Chloroethane	49
Chloroform	52
Cyclohexane	55
Di-n-butyl phthalate	58
1,1-Dichloroethane	60
1,2-Dichloroethane	63
1,1-Dichloroethene	66
trans-1,2-Dichloroethene	69
Dimethyl sulfoxide	71
1,4-Dioxane	74
Ethanol	77
Ethylbenzene	81
Ethylene dibromide	84
Methanol	87
Methylene chloride	91
Naphthalene	94
Phenol	97
Quinoline	101
Tetrachloroethene	103
Toluene	106
1,1,1-Trichloroethane	109
Trichloroethene	112
Vinyl chloride	115
Water	118
m-Xylene	121
o-Xylene	124
p-Xylene	127
References and Bibliography	130

SUMMARY TABLES

page

1. Ranking of top 20 organic ground water contaminants based on number of sites at which each contaminant was detected. 17

2. Selected toxic organic chemicals ordered by Chemical Abstract Service Registry Number (CAS RN). Those chemicals on the U.S. EPA top 100 hazardous substances list are also noted. 18

3. Selected toxic organic chemicals ordered by number of carbon and hydrogen atoms. 19

4. Ranking of selected toxic organic chemicals by specific gravity at room temperature. 20

5. Solubilities of selected toxic organic chemicals. 21

6. Vapor pressure and boiling point of selected toxic organic chemicals and water. Ranking by vapor pressure. 22

7. Relative dielectric permittivities for selected toxic organic chemicals and water. 23

8. Ranking of selected organic chemicals by ionization potential. 24

9. Ranking of selected toxic organic chemicals by fire hazard. 25

10. Threshold limit exposure values for selected toxic chemicals. 26

INTRODUCTION

This report summarizes information on physical, chemical and thermodynamic properties, uses, fire and explosion hazards, health hazards, and handling precautions for thirty-three toxic organic chemicals. Twenty of these are some of the most commonly occurring organic ground water contaminants found at hazardous waste disposal sites (Plumb and Pitchford, 1985). Twenty-five are on the U.S. Environmental Protection Agency top 100 hazardous substances list. The data were compiled from handbooks, texts, and reports listed in the annotated Reference and Bibliography section. References are noted by brackets following the numeric data. Though twenty references were used as sources for the physical property data, Dean (1985), Weast (1985) and Riddick, et al. (1986) accounted for about 60% of the data. Another 25% of the information was taken from Gray (1972), Perry and Chilton (1973), Mackison, et al. (1981), Sax (1984) and Weiss (1986). The remainder of the data was taken from the other references noted. Care was taken to include all available data in an accurate and concise format. Definitions for all properties and conversion factors are discussed in the first section of this report. Synonyms, including tradenames as well as common or generic names that can be ambiguously applied to given substances, are supplied. Fire and explosion hazards are briefly summarized in terms of explosive limits, flash points, and incompatible materials. The various uses of the chemicals are also included. The Chemical Abstract Service Registry Number (CAS RN) is provided for positive identification of each chemical.

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), Mackison et al. (1981), Verschueren (1983), Sax (1984) and Baker Chemical Co. (1986). 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 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, Bretherick, 1981, and material safety data sheets) should be referred to for first aid procedures. All chemicals should be disposed of in accordance with all applicable federal, state and local environmental regulations. Contact local health and pollution control agencies for proper and legal disposal procedures.

The toxic chemicals in this report appear in alphabetic sequence. Water is included for reference and as a standard for calibration and comparison. Tables that summarize and compare various properties of the chemicals appear near the beginning of the report. An annotated Reference and Bibliography section is included that lists relevant sources in addition to those cited as references.

The data and information compiled in this report represent a portion of the initial phase of the Toxic Waste Geophysics investigations being conducted by the the U.S. Geological Survey. The author is not aware of any other single document that presents such a comprehensive list of properties for the selected chemicals. In the future, this list will be expanded as necessary and will be available in computer format for easy access. One purpose in compiling this report is to define data "gaps" concerning physical properties, electrochemical properties and clay-organic interactions of these chemicals. 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. A much more thorough literature search is planned before the next update of this report is published. The author encourages readers to contribute new data concerning these chemicals and to correct any errors. The report is intended to be used principally by the laboratory investigator. However, it also may be useful to field engineers and to others involved with hazardous chemical waste management and studies.

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THE PROPERTIES

This section contains brief discussions of the physical and chemical properties described in this report. A list of abbreviations and a conversion table from SI to cgs and English systems is also included. Property values are reported in SI units except where temperature is referred to in degrees Celsius for convenience. Definitions were compiled from various references.

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.

Boiling point. 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.

Ceiling limit (CL). ACGIH TLV value. This limit is a concentration (in ppm) 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 approximately one atmosphere. Units are reciprocal pascals (Pa^{-1}).

Contact angle. The angle a liquid drop of a substance makes on a specified substrate. The smaller the angle (in degrees) the more spherical the shape of the drop.

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.

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.

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 (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) per 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 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 chemical 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. Methods used are open cup (OC) or closed cup (CC) at one atmosphere pressure.

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 kilojoule 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. Latent heat is not accompanied by a change in temperature.

Heat capacity. The quantity of heat required to raise a liquid chemical system one degree in temperature, at 25^{o}C and constant pressure. Given in kilojoule 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 kilojoule 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 kilojoule 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 kilojoule per mole (kJ/mol).

Heat of polymerization. The amount of heat released when the compound (or monomer) polymerizes to form the polymer. A negative value indicates heat is given off. Given in kilojoule per mole (kJ/mol).

Heat of solution. The heat evolved or absorbed when a substance is dissolved in water at a given temperature. A negative value indicates heat is given off. Given in kilojoule 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 kilojoule per mole (kJ/mol).

Heat of vaporization. The heat required to convert one mole of a liquid to the gaseous state with no temperature change. Given in kilojoule per mole (kJ/mol).

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; PI - photoionization; S - optical spectroscopy.

Kinematic viscosity. The ratio of the dynamic viscosity to the density of a fluid. Given in micro-meter squared per second ($\mu m^2/s$). 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, ie., the energy loss per cycle in a dielectric material due to conduction and slow polarization currents or other dissipative effects (such as elastic relaxation). Also referred to as the dielectric dissipation factor.

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

Mole (mol). The amount of pure substance containing Avogadro's number of atoms (i.e., 6.022045×10^{23}), 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 or 0.5551 mol, where 18.0152 is the relative molecular mass of H_2O.

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.

Partition coefficient. A measure of the distribution of a given compound in two phases and expressed as a concentration ratio, assuming no interactions other than simple dissolution. Partition coefficients are valuable in describing the environmental behavior of compounds. Kow is the octonal/water partition coefficient. Koc is the soil/water partition coefficient.

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. For example, pure water dissociates to H^+ and OH^- with a concentration of H^+ of 1×10^{-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. The pK is frequently used to express the extent of dissociation, or the strength, of weak acids, the pKa (or acid dissociation constant) . The weaker the electrolyte the larger its pKa. Strong acids will have values <5, and weak acids will have values >5 for their pKa. 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 pKs is the negative log of the autoprotolysis constant of a solvent employed in nonaqueous acid-base titrations in 0.01M solution. The pKh is the negative logarithm of the ionization constant of a protonated base.

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

Relative dielectric permittivity. The dielectric permittivity of a substance relative to that of vacuum (sometimes called dielectric constant). The real part of the relative complex permittivity. Permittivity is that property of a material which resists the transmission of an electrostatic force from one charged body to another. It is a measure of the capacity of a material to store charge when an electric field is applied. The lower the dielectric permittivity of a substance is, the higher the electrical resistance will be.

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. The calculation of relative molecular masses was made using the following values from [85]. Bromine=79.904, Carbon=12.011, Chlorine=35.453, Hydrogen=1.00794, Nitrogen=14.0067, Oxygen=15.9994, 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 = 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 the chemicals to be dissolved in various solvents. It is described as follows: insoluble (0 %), slightly soluble (<5 %), soluble (5-50 %), very soluble (>50 %), miscible (100 %).

Solution diffusivity. The rate of diffusion of dilute solutions of the listed solute in various solvents at one atmospheric pressure, in nano-meter squared per second (nm^2/s).

Specific gravity. At 20/4, i.e., the dimensionless ratio of the density of the substance, at 20°C, to the density of water at 4°C, or as noted, and one atmospheric 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.

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 milli-newtons per meter (mN/m).

Synonyms (syn). Includes common, trivial, and commercial names. Some common names may be ambiguously applied.

Thermal conductivity. The quantity of heat conducted per unit time through unit area of unit thickness 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 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) and represent a "threshold" dose below which there are no known adverse effects. These exposure guidelines were developed by the American Conference of Governmental Industrial Hygienists (ACGIH). 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.

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

Vapor pressure. The 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.

Volume susceptibility. The magnetic volume susceptibility. A dimensionless quantity. 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. All of the substances in this report with listed susceptibilities are called diamagnetic, that is, their magnetic susceptibilities are negative.

ABBREVIATIONS

A	ampere, base SI unit of electric current
ACGIH	American Conference of Governmental Industrial Hygienists
ANSI	American National Standards Institute
atm	standard atmosphere, a unit of pressure
Autoign. temp.	autoignition temperature
b	bar, unit of pressure (of fluid)
Btu	British thermal unit
C	coulomb, s-A, SI unit of electric charge, electric flux and elementary charge
^{o}C	degree Celsius, SI unit of Celsius temperature and temperature interval
cal	calorie, thermochemical; also called gram calorie
(CC)	closed cup flash point tetser, kind not specified
CL	OSHA ceiling limit for human exposure
C-m	coulomb-meter
cm	centimeter
CNS	central nervous system
cP	centipoise
cSt	centistoke
D	Debye unit of dipole moment
dm	decimeter
dyn	dyne, g-cm/s^2, 10^{-5} N, cgs unit of force
eV	electron volt, unit of energy
(EI)	electron impact method to measure ionization potential
^{o}F	degree Fahrenheit, unit of Fahrenheit temperature and temperature interval
ft	foot
ft-lbf	foot pound-force
g	gram
(gas)	gaseous or vapor phase
Hg	mercury
hr	hour
IDLH	immediately dangerous to life and health value
in	inch
J	joule, m^2kg-s, N-m, Pa-m^3, 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
kJ	kilojoule
Koc	soil/water partition coefficient
Kow	octonal/water partition coefficient
kPa	kilopascal

l,L	liter or litre
lel	lower explosion limit
(liq)	liquid phase
M	molarity, one molar concentration
m	meter, base SI unit of length
mg	milligram
min	minute
mL	milliliter
mm	millimeter
mN	millinewton
MOhm-m	megohm-meter
mol	mole, base SI unit of amount of substance
mPa	millipascal
MPa	megapascal
N	newton, kg-m/s^2, SI unit of force and 'weight'
NA	data not available or not applicable
NIOSH	National Institute for Occupational Safety and Health
nm	nanometer
nPa	nanopascal
(OC)	open cup flash point tester, kind not specified
OSHA	Occupational Safety and Health Administration
oz	ounce
P	poise, dyn-s/cm^2, cgs unit of (dynamic) viscosity
Pa	pascal, N/m^2, $m^{-1}kgs^{-2}$, J/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
pKa	negative logarithm of acid dissociation constant
pKh	negative logarithm of ionization constant of a protonated base
pKs	negative logarithm of autoprotolysis constant
ppm	parts per million
psi	pound per square inch, correctly: pound-force per square inch (lbf/in^2)
PVA	polyvinyl alcohol
PVC	polyvinyl chloride
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^2/s, cgs unit of kinematic viscosity
STEL	short term exposure limit
Syn	synonyms
TLV	threshold limit value

TWA	time-weighted average exposure limit
uel	upper explosion limit
μg	microgram
μm	micrometer
V	volt, SI unit of electric potential, potential difference and electromotive force
W	Watt, m^2kg/s^3, J/s, SI unit of power
>>	very much greater than
>	greater than
=	equal to
<	less than
<<	very much less than

CONVERSION FACTORS

Concentration:
ppm = (mg/m^3) * 24.45/relative molecular mass
mg/m^3 = ppm * relative molecular mass/24.45

Density:
1 g/cm^3 = 1000 kg/m^3 = 0.0361273 lb/in^3 = 62.428 lb/ft^3

Dipole moment:
1 Debye = 3.33564 * 10^{-30} coulomb-meter
1 coulomb = 1 second-ampere = 2.77778 * 10^{-4} Amp-hr

Energy, Heat or Work:
1 cal = 4.1868 J = 1.163 * 10^{-6} kW-hr = 3.96832 * 10^{-3} Btu
1 eV = 1.6021892 * 10^{-19} J
1 Btu = 1055.06 J = 2.930 * 10^{-4} kW-hr = 778.169 ft-lbf
1 J = 9.47817 * 10^{-4} Btu = 0.238846 cal = 1 * 10^7 erg

3
Length:
1 m = 3.28084 ft = 39.3701 in
1 in = 2.540 cm
1 Angstrom unit = 1 * 10^{-10} m = 0.1 nm

Mass:
1 lb = 16 oz = 453.59237 g

Pressure:
1 atm = 760.002 mm Hg = 0.1013274 MPa = 14.6960 psi
1 mm Hg = 1 torr = 133.322 Pa = 0.133322 kPa = 51.715 psi
1 MPa = 9.86923 atm = 145.038 psi
1 dyn/cm^2 = 0.1 Pa

Surface tension:
1 dyn/cm = 0.001 N/m = 1 mN/m

Susceptibility:
1 SI unit = 4 π cgs units

Temperature:
$^oF = (1.8 * {}^oC)+32$
$^oC = ({}^oF-32)/1.8$
$K = {}^oC+273.15 = ({}^oF+459.67)/1.8$

Thermal conductivity:
1 cal/(s-cm-K) = 418.68 W/(m-K)
1 Btu/(hr-ft-^{o}F)= 1.73073 W/(m-K)

Viscosity:
1 cP = 0.001 kg/(m-s) = 0.001 Pa-s = 1 mPa-s
1 cSt = 0.000001 m^2/s

Volume:
1 L = 0.001 m^3 = 1 dm^3 = 1000 cm^3 = 1.0566881 liquid quart

Table 1. 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.

Rank	Substance	Molecular formula
1	Trichloroethene	C_2HCl_3
2	Methylene chloride	CH_2Cl_2
3	Tetrachloroethene	C_2Cl_4
4	Toluene	C_7H_8
5	1,1-Dichloroethane	$C_2H_4Cl_2$
6	Bis(2-ethylhexyl)phthalate	$C_{24}H_{38}O$
7	Benzene	C_6H_6
8	trans-1,2-Dichloroethene	$C_2H_2Cl_2$
9	1,1,1-Trichloroethane	$C_2H_3Cl_3$
10	Chloroform	$CHCl_3$
11	Ethylbenzene	C_8H_{10}
12	1,2-Dichloroethane	$C_2H_4Cl_2$
13	1,1-Dichloroethene	$C_2H_2Cl_2$
14	Phenol	C_6H_6O
15	Vinyl chloride	C_2H_3Cl
16	Chlorobenzene	C_6H_5Cl
17	Di-n-butyl phthalate	$C_{16}H_{22}O_4$
18	Naphthalene	$C_{10}H_8$
19	Chloroethane	C_2H_5Cl
20	Acetone	C_3H_6O

Table 2. Selected toxic organic chemicals ordered by Chemical Abstract Service Registry Number (CAS RN). Those chemicals on the U.S. Environmental Protection Agency top 100 hazardous substances list are also noted by a number indicating which of the priority groups they are in. Each priority groups consist of 25 substances. Group 1 has the highest priority.

CAS RN	Substance	Priority Group
56235	Carbon tetrachloride	2
64175	Ethanol	
64197	Acetic acid	
67561	Methanol	
67641	Acetone	
67663	Chloroform	1
67685	Dimethyl sulfoxide	
71432	Benzene	1
71556	1,1,1-Trichloroethane	3
75003	Chloroethane	2
75014	Vinyl chloride	1
75092	Methylene chloride	1
75252	Bromoform	3
75343	1,1-Dichloroethane	3
75354	1,1-Dichloroethene	2
79016	Trichloroethene	1
84742	Di-n-butyl phthalate	3
91203	Naphthalene	3
91225	Quinoline	
95476	o-Xylene	3
100414	Ethylbenzene	3
106423	p-Xylene	3
106934	Ethyl dibromide	
107062	1,2-Dichloroethane	2
108383	m-Xylene	3
108883	Toluene	2
108907	Chlorobenzene	3
108952	Phenol	2
110827	Cyclohexane	
117817	Bis(2-ethylhexyl)phthalate	1
123911	1,4-Dioxane	4
127184	Tetrachloroethene	1
156605	trans-1,2-Dichloroethene	3

Table 3. Selected toxic organic chemicals ordered by number of carbon and hydrogen atoms. Most common synonyms are also noted.

Formula	Substance
CCl_4	Carbon tetrachloride, tetrachloromethane,
$CHBr_3$	Bromoform, tribromethane, methyl tribomide
$CHCl_3$	Chloroform, trichloromethane, methane trichloride
CH_2Cl_2	Methylene chloride, methane dichloride, dichloromethane
CH_4O	Methanol, methyl alcohol, wood spirit
C_2Cl_4	Tetrachloroethene, perchloroethylene, ethylene tetrachloride
C_2HCl_3	Trichloroethene, ethylene trichloride
$C_2H_2Cl_2$	1,1-Dichloroethene, vinylidene chloride
$C_2H_2Cl_2$	trans-1,2-Dichloroethene, acetylene dichloride
C_2H_3Cl	Vinyl chloride, chloroethylene
$C_2H_3Cl_3$	1,1,1-Trichloroethane, methyl chloroform, chloroethene
$C_2H_4Br_2$	Ethylene dibromide, 1,2-dibromoethane, ethylene bromide
$C_2H_4Cl_2$	1,1-Dichloroethane, ethylidene chloride
$C_2H_4Cl_2$	1,2-Dichloroethane, ethylene dichloride
$C_2H_4O_2$	Acetic acid, ethanoic acid, vinegar acid
C_2H_5Cl	Chloroethane, ethyl chloride
C_2H_6O	Ethanol, ethyl alcohol, anhydrous alcohol, grain alcohol
C_2H_6OS	Dimethyl sulfoxide, DMSO, methyl sulfoxide
C_3H_6O	Acetone, propanone
$C_4H_8O_2$	1,4-Dioxane, diethylene oxide, 1,4-dioxacyclohexane
C_6H_5Cl	Chlorobenzene, benzene chloride, phenyl chloride
C_6H_6	Benzene, benzol
C_6H_6O	Phenol, carbolic acid, hydroxybenzene
C_6H_{12}	Cyclohexane, hexahydrobenzene, hexanaphthalene, hexamethalene
C_7H_8	Toluene, methylbenzene, phenylmethane
C_8H_{10}	Ethylbenzene, phenylethane
$o\text{-}C_8H_{10}$	o-Xylene, 1,2-dimethylbenzene, o-methyltoluene
$m\text{-}C_8H_{10}$	m-Xylene, 1,3-dimethylbenzene, m-methyltoluene
$p\text{-}C_8H_{10}$	p-Xylene, 1,4-dimethylbenzene, p-methyltoluene
C_9H_7N	Quinoline, 1-benzanine, 1-azanaphthalene
$C_{10}H_8$	Naphthalene, tar camphor
$C_{16}H_{22}O_4$	Di-n-butyl phthalate, dibutyl phthalate
$C_{24}H_{38}O_4$	Bis(2-ethylhexyl)phthalate, dioctyl phthalate

Table 4. Ranking of selected toxic organic chemicals by specific gravity at room temperature. Values less than 1.0 indicate substance will float on water.

Substance	Specific gravity	
Cyclohexane	0.77855	
Ethanol	0.7893	
Acetone	0.7899	
Methanol	0.7914	
p-Xylene	0.8611	
m-Xylene	0.8642	
o-Xylene	0.8802	
Toluene	0.8669	
Ethylbenzene	0.8670	
Benzene	0.8765	
Chloroethane	0.8979	
Vinyl chloride	0.9106	
Bis(2-ethylhexyl)phthalate	0.9843	floaters
Water	1.0000	
1,4-Dioxane	1.0337	sinkers
Di-n-butyl phthalate	1.047	
Acetic acid	1.0492	
Phenol	1.0576	
Quinoline	1.0929	
Dimethyl sulfoxide	1.10041	
Chlorobenzene	1.1058	
Naphthalene	1.162	
1,1-Dichloroethane	1.1757	
1,1-Dichloroethene	1.2129	
1,2-Dichloroethane	1.253	
trans-1,2-Dichloroethene	1.2565	
Methylene chloride	1.3266	
1,1,1-Trichloroethane	1.3390	
Trichloroethene	1.4642	
Chloroform	1.4832	
Carbon tetrachloride	1.5940	
Tetrachloroethene	1.6227	
Ethylene dibromide	2.1792	
Bromoform	2.8899	

Table 5. Solubilities of selected toxic organic chemicals in water, ethanol, ethyl ether, acetone and benzene. Actual values when given are in grams per 100 grams of solvent at room temperature. (Alc=ethanol).

M	Miscible	100 %
V	Very Soluble	> 50 %
So	Soluble	5-50 %
Sl	Slightly Soluble	< 5 %
I	Insoluble	0 %
-	No data	

Substance	Water	Alc	Ether	Acetone	Benzene
Acetic acid	M	M	M	M	M
Acetone	M	M	M	M	M
Benzene	0.70	M	M	M	M
Bis(2-ethylhexyl)phthalate	0.01	-	-	-	-
Bromoform	0.1	M	M	-	So
Carbon tetrachloride	0.08	M	M	M	M
Chlorobenzene	0.05	M	M	-	V
Chloroethane	0.57	48.3	M	-	-
Chloroform	0.82	M	M	So	M
Cyclohexane	0.01	M	M	M	M
Di-n-butyl phthlate	0.45	V	V	V	V
1,1-Dichloroethane	0.50	V	V	So	So
1,2-Dichloroethane	0.90	V	M	So	-
1,1-Dichloroethene	0.021	So	V	So	So
trans-1,2-Dichloroethene	0.35	M	M	M	-
Dimethyl sulfoxide	25.3	So	So	So	So
1,4-Dioxane	M	M	M	M	M
Ethanol	M	M	M	M	So
Ethylbenzene	0.015	So	V	M	M
Ethylene dibromide	0.43	M	M	So	So
Methanol	M	M	M	M	M
Methylene chloride	1.32	M	M	-	-
Naphthalene	0.003	9.5	57.12	69.16	46
Phenol	8.2	V	V	-	8.2
Quinoline	0.6	M	M	M	M
Tetrachloroethene	0.015	M	M	-	M
Toluene	0.05	M	M	So	M
1,1,1-Trichloroethane	0.07	M	M	So	So
Trichloroethene	0.1	M	M	So	-
Vinyl chloride	0.27	So	V	-	So
m-Xylene	0.00003	M	M	M	M
o-Xylene	0.00003	M	M	M	M
p-Xylene	0.00003	M	M	M	M
Water	M	M	1.468	M	0.635

Table 6. Vapor pressure at 20°C (or as noted) and boiling point (B.P.) in degrees Celsius of selected toxic organic chemicals and water. Substances are ranked by vapor pressure which is proportional to volatility. Atmospheric pressure (at sea level) is approximately 101.325 kPa or 760 mm Hg.

Substance	20°C Vapor Pressure kPa (mm Hg)	B.P. °C
Vinyl chloride	337.3 (2530)	-13.37
Chloroethane	141.8 (1064)	12.3
1,1-Dichloroethene	66.67 (500)	31.7
Methylene chloride	46.66 (350)	40.2
trans-1,2-Dichloroethene	35.33 (265)	47.5
1,1-Dichloroethane	24.26 (182)	57.3
Acetone	24.24 (182)	56.2
Chloroform	21.33 (160)	61.2
1,1,1-Trichloroethane	13.33 (100)	74.0
Methanol	12.93 (97)	64.5
Cyclohexane	12.7 (95)	80.7
Carbon tetrachloride	12.13 (91)	76.6
Benzene	10.13 (76)	80.1
1,2-Dichloroethane	8.13 (61)	83.5
Trichloroethene	7.73 (58)	87.2
Ethanol	5.33 (40) @ 19°C	78.3
1,4-Dioxane	3.87 (29)	101.3
Toluene	2.93 (22)	110.6
Water	2.3378 (17.535)	100.0
Tetrachloroethene	1.87 (14)	121.2
Acetic acid	1.52 (11.4)	118.1
Ethylene dibromide	1.47 (11)	131.4
p-Xylene	1.20 (9)	138.4
m-Xylene	1.20 (9)	139.1
Chlorobenzene	1.17 (8.8)	132.0
Ethylbenzene	0.947 (7.1)	136.2
o-Xylene	0.933 (7.0)	144.4
Bromoform	0.667 (5.0)	149.5
Dimethyl sulfoxide	0.0493 (0.37)	189.0
Phenol	0.0480 (0.36)	181.8
Naphthalene	0.0067 (0.05)	218.0
Quinoline	0.0112 (0.84) @ 25°C	237.1
Di-n-butyl phthalate	<0.0013 (<0.01)	340
Bis(2-ethylhexyl)phthalate	0.160 (1.2) @ 200°C	384

Table 7. Relative dielectric permittivity (dielectric constant) for selected toxic organic chemicals and water. Substances are liquid unless noted otherwise. Relative permittivity of the chemicals is useful in predicting electrical property changes in groundwater, soils, etc., in the case of a spill or other discharge.

Substance	relative permittivity	temp, °C
Vacuum	1.000	
Air (dry, CO_2 free)	1.000537	20
Cyclohexane	2.024	20
trans-1,2-Dichloroethene	2.14	25
1,4-Dioxane	2.209	25
Carbon tetrachloride	2.238	20
p-Xylene	2.27	20
Benzene	2.284	20
Tetrachloroethene	2.30	25
m-Xylene	2.374	20
Toluene	2.379	25
Ethylbenzene	2.412	20
Naphthalene (solid - 400 MHz)	2.52	17-22
Naphthalene	2.54	85
o-Xylene	2.568	20
Trichloroethene	3.42	16
Phenol (solid - 400 MHz)	4.3	10
Bromoform	4.39	20
1,1-Dichloroethene	4.67	16
Ethylene dibromide	4.78	25
Chloroform	4.806	20
Bis(2-ethylhexyl)phthalate	5.3	20
Chlorobenzene	5.71	20
Acetic acid	6.15	20
Vinyl chloride	6.26	17.2
Di-n-butyl phthalate	6.436	30
1,1,1-Trichloroethane	7.68	20
Quinoline	9.0	25
Methylene chloride	9.08	20
Chloroethane	9.45	20
Phenol	9.78	60
1,1-Dichloroethane	10.0	18
1,2-Dichloroethane	10.36	25
Acetone	21.45	20
Ethanol	25.07	20
Methanol	33.64	20
Dimethyl sulfoxide	46.45	25
Water	80.18	20

Table 8. Ranking of selected organic chemicals by ionization potential. The ionization potential is used by various instruments to test atmospheres for the presence of toxic substances.

Substance	Ionization potential (eV)
Water	12.6
Carbon tetrachloride	11.47
Chloroform	11.42
Methylene chloride	11.35
1,2-Dichloroethane	11.12
Chloroethane	10.97
Methanol	10.84
Bromoform	10.51
Ethanol	10.49
Acetic acid	10.37
Vinyl chloride	9.996
Cyclohexane	9.8
Acetone	9.69
trans-1,2-Dichloroethene	9.64
Trichloroethene	9.45
Ethylene dibromide	9.45
Tetrachlorethene	9.32
Benzene	9.24
1,4-Dioxane	9.13
Chlorobenzene	9.07
Toluene	8.82
Ethylbenzene	8.76
m-Xylene	8.58
o-Xylene	8.56
Phenol	8.51
p-Xylene	8.44
Naphthalene	8.12

Table 9. Ranking of selected toxic organic chemicals by fire hazard. Rating based primarily on flash points then explosive ranges in air. Toluene is the exception as it is not very flammable despite low flash point. Ratings were determined generally as follows: Very high - flash point < 0°C (32°F); High - flash point between 0°C and 38°C (100°F), Moderate - flash point between 38°C and 93°C (200°F), Low - flash point > 93°C, Very low - non-combustible (NC).

Substance	Flash point °C	lel %	uel %	Rating
Vinyl chloride	-78	3.6	22.0	Very high
Chloroethane	-50	3.8	15.4	Very high
1,1-Dichloroethene	-18	7.3	16.0	Very high
Cyclohexane	-20	1.33	8.4	Very high
Acetone	-18	2.6	12.8	Very high
Benzene	-11	1.4	8.0	Very high
1,1-Dichloroethane	-5.6	0.9	5.9	Very high
trans-1,2-Dichloroethene	2.2	9.7	12.8	High
Methanol	12.2	6.0	36.5	High
1,4-Dioxane	12.2	2	22	High
Ethanol	13.1	3.3	19	High
1,2-Dichloroethane	12.8	6.2	15.6	High
Ethylbenzene	15	1	6.7	High
Xylenes	29	1.1	6.4	High
Chlorobenzene	28.9	1.3	7.0	High
Acetic acid	43	5.4	16	Moderate
Phenol	79.4	1.7	8.6	Moderate
Naphthalene	78.9	0.9	5.9	Moderate
Toluene	4.4	1.27	7.0	Moderate
Dimethyl sulfoxide	95	2.6	28.5	Low
Quinoline	107.2	NA	NA	Low
Di-n-butyl phthalate	157	0.5	2.5	Low
Bis(2-ethylhexyl)phthalate	218	NA	NA	Low
Methylene chloride	NC			Very Low
Chloroform	NC			Very low
Trichloroethene	NC			Very low
1,1,1-Trichloroethane	NC			Very low
Tetrachloroethene	NC			Very low
Carbon tetrachloride	NC			Very low
Bromoform	NC			Very low
Ethylene dibromide	NC			Very low

Table 10. Threshold limit values and IDLH values for selected organic air contaminants. Each of these values may have not been determined for every chemical listed. For many carcinogens only TWAs are available because short term effects are often minor. Carcinogens and suspected carcinogens are noted by an asterisk in the last column under "C".

Substance	TWA ppm	STEL ppm	CL ppm	IDLH ppm	C
Quinoline	0.1				
Bis(2-ethylhexyl)phthalate	0.3				*
Di-n-butyl phthlate	0.5				
Bromoform	0.5				
Vinyl chloride	1		5		*
1,1-Dichloroethene	1		5		*
Phenol	5	10		100	
Carbon tetrachloride	5		25		*
Acetic acid	10	15	20	1000	
Benzene	10	25	25	2000	*
1,2-Dichloroethane	10		100	1000	*
Chloroform	10		50	1000	*
Naphthalene	10	15		500	
Ethylene dibromide	20		30	400	*
1,4-Dioxane	25			200	*
Trichloroethene	50	200	150	1000	*
Tetrachloroethene	50	200	200	500	
Chlorobenzene	75			2400	
Methylene chloride	100		1000	5000	
Toluene	100	150	200	2000	
1,1-Dichloroethane	100	250			
Ethylbenzene	100	125		2000	
Xylenes	100	150	200		
Methanol	200	250	600	25000	
trans-1,2-Dichloroethene	200	250		4000	
Cyclohexane	300	375		10000	
1,1,1-Trichloroethane	350	450	350	1000	
Acetone	750	1000	3000	20000	
Ethanol	1000				
Chloroethane	1000				

ACETIC ACID $C_2H_4O_2$ CAS RN: 64197

Syn: Glacial acetic acid; ethanoic acid; ethylic acid; methane carboxylic acid; vinegar acid.

Chemical formula: CH_3COOH Carboxylic Acid

Physical properties:

Relative molecular mass:	60.0526	
Specific gravity:	1.0492	[8]
Boiling point:	118.1°C	[8]
Melting point:	16.6°C	[8]
Refractive index:	1.3719	[8]
Vapor pressure:	1.520 kPa @ 20°C	[63]
Vapor density:	2.07	[63]
Evaporation rate:	0.97	[37]
Relative permittivity:	6.15 @ 20°C	[85]
	6.29 @ 40°C	[85]
	6.62 @ 70°C	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.172 W/(m-K) @ 20°C	[85]
	0.180 @ 25°C	[8]
Electrical resistivity:	200 MOhm-m @ 0°C	[8]
	89.3 @ 25°C	[8]
Critical temperature:	319.56°C	[58]
Critical pressure:	5.786 MPa	[58]
Dynamic viscosity:	1.314 mPa-s @ 15°C	[8]
	1.30 @ 18°C	[85]
	1.155 @ 25.2°C	[85]
	1.04 @ 30°C	[85]
	1.00 @ 41°C	[85]
	0.70 @ 59°C	[85]
	0.60 @ 70°C	[85]
	0.43 @ 100°C	[85]
Kinematic viscosity:	1.252 $\mu m^2/s$ @ 15°C	
	1.24 @ 18°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	[85]
	27.8 @ 20°C vapor	[85]
	26.34 @ 30°C	[12]
	24.8 @ 50°C vapor	[85]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.001078 K^{-1} @ 20°C	[58]
	0.00111 @ 55°C	[58]

Compressibility:	0.875 nPa^{-1}	@ 15°C	[85]
	0.908	@ 20°C	[85]
	0.972	@ 30°C	[85]
	1.037	@ 40°C	[85]
	1.111	@ 50°C	[85]
	1.191	@ 60°C	[85]
	1.277	@ 70°C	[85]
	1.368	@ 80°C	[85]
Vapor diffusivity:	10.64 $\mu m^2/s$	@ 0°C	[52]
Solution diffusivity:	3.31 nm^2/s	in Acetone	[52]
	2.11	in Benzene	[52]
	1.49	in CCl^4	[52]
	0.13	in Ethylene glycol	[52]
	2.26	in Toluene	[52]
	1.24	in Water	[52]
Electric dipole moment:	5.804 x 10^{-30} C-m		[85]
Ionization potential:	NA		
Volume susceptibility:	-6.92 x 10^{-6} SI units	@ 32°C	[85]
Speed of sound:	NA		
Heat of melting:	11.723 kJ/mol		[8]
Heat of vaporization:	23.710 kJ/mol		[8]
Heat of sublimation:	NA		
Heat capacity @ 25°C:	0.1243 kJ/ (mol-K)	(liq)	[8]
	0.0666	(gas)	[8]
Heat of combustion:	-875.1 kJ/mol	@ 25°C (liq)	[85]
Heat of formation:	-484.5 kJ/mol	@ 25°C (liq)	[8]
	-435.1	(gas)	[8]
Gibbs (free) energy:	-390.2 kJ/mol	@ 25°C (liq)	[8]
	-376.9	(gas)	[8]

Analytical chemistry:	pKs = 1.5		[8]
	pKa = 4.76	@ 20-35°C in Water	[8]
	9.52	in Methanol	[8]
	10.32	in Ethanol	[8]
	11.4	in Dimethyl sulfoxide	[8]
	9.75	in Acetone+10% Water	[8]

Electrochemical data : [33], [38], [70], [77].

Clay-organic interaction data: 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. [75]

Solubility: Miscible with water, ethanol, ether, acetone, and benzene, n-heptane, carbon tetrachloride.

Form: Colorless liquid or solid; pungent vinegar-like odor.

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 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.

Fire and Explosion Hazard: Moderate.
Flash point: 43°C (CC) [63]
lel: 5.4% @ 100°C [63]; uel: 16.0% @ 100°C [63]
Autoign. temp.: 465°C [63]
Combustible liquid. Moderate fire and explosion hazard when exposed to heat, sparks or flame. Dangerous, as toxic gases and vapors (such as carbon monoxide) may be released in a fire. Can react vigorously with oxidizing materials. Fight fire with CO_2, dry chemical, alcohol foam or water spray.

Incompatible: With chromic acid, 5-azidotetrazole, hydrogen peroxide, sodium peroxide, nitric acid, acetaldehyde, 2-amino-ethanol, NH_4NO_3, BrF_5, ClF, chlorosulfonic acid, (O_3+diallyl methyl carbinol), ethylenediamine, ethylene imine, H_2O_2, (HNO_3+acetone), potassium-tert-butoxide, oleum, $HClO_4$, permanganates, $P(OCN)_3$, PCl_3, KOH, NaOH, n-xylene, strong bases. Liquid will attack many synthetic resins or rubber.

Handling: Avoid heat, sources of ignition and flame. Prevent skin contact or inhalation (rubber, neopren, latex or nitrile gloves, lab coat and apron, safety goggles, face shield, body shield). Use in well ventilated area (fume hood). Store in cool, dry well-ventilated flammable liquid storage area or cabinet.

Health Effects: Acetic acid 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. Swallowing concentrated solutions may cause severe injury or death.

Toxicity: Moderate.
TWA: 10 ppm
STEL: 15 ppm
CL: 20 ppm
IDLH: 1000 ppm
Peak: 40 ppm for 5 min
Odor threshold: 0.2-24 ppm
Exposure: Nasal irritation occurs at 10 to 12 ppm, with extreme eye and nasal irritation at concentrations in excess of 25 ppm. Effects at 50 ppm are intolerable. Acclimatized workers exposed to 80 to 200 ppm for 7 to 12 years 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.
External: 50 mg/24 hr--mild skin irritation
Oral:
Non-lethal: 1470 μg/kg
1 mL--Perforation of the esophagus
Inhalation:
Non-lethal: 816 ppm/3 min

ACETONE C_3H_6O CAS RN: 67641

Syn: 2-Propanone; dimethyl ketone; B-ketopropane; ketone propane; propanone dimethylformaldehyde; dimethylketal; pyroacetic acid; pyroacetic ether.

Chemical formula: CH_3COCH_3 Aliphatic Ketone

Physical properties:

Relative molecular mass:	58.0798	
Specific gravity:	0.7899	[85]
Boiling point:	56.2°C	[85]
Melting point:	-94.8°C	[85]
Refractive index:	1.3588	[85]
Vapor pressure:	24.227 kPa @ 20°C	[58]
Vapor density:	2.00	[63]
Evaporation rate:	5.59	[58]
Relative permittivity:	20.9 @ 20°C	[58]
	20.7 @ 25°C	[85]
	17.7 @ 56°C	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.177 W/(m-K) @ -20°C	[20]
	0.169 @ 0°C	[20]
	0.162 @ 20°C	[20]
	0.155 @ 40°C	[20]
Electrical resistivity:	0.5 MOhm-m @ 18°C	[8]
	0.1667 @ 25°C	[8]
Critical temperature:	236.5°C	[8]
Critical pressure:	4.783 MPa	[8]
Dynamic viscosity:	0.450 mPa-s @ -10°C	[85]
	0.399 @ 0°C	[85]
	0.337 @ 15°C	[85]
	0.316 @ 25°C	[85]
	0.295 @ 30°C	[85]
	0.280 @ 41°C	[85]
Kinematic viscosity:	0.569 $\mu m^2/s$ @ -10°C	
	0.505 @ 0°C	
	0.427 @ 15°C	
	0.400 @ 25°C	
	0.373 @ 30°C	
	0.354 @ 41°C	
Surface tension:	26.21 mN/m @ 0°C air, vapor	[85]
	23.70 @ 20°C air, vapor	[85]
	22.68 @ 25°C	[58]
	22.01 @ 30°C	[58]
	21.16 @ 40°C air, vapor	[85]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.00143 K^{-1}	[58]
Compressibility:	1.229 nPa^{-1} @ 20°C	[85]
	1.334 @ 30°C	[85]
	1.464 @ 40°C	[85]

Vapor diffusivity:	10.9 $\mu m^2/s$ @ 0°C		[52]
Solution diffusivity:	NA		
Electric dipole moment:	9.61 x 10^{-30} C-m		[8]
Ionization potential:	9.69 eV (PI)		[85]
Volume susceptibility:	-5.8 x 10^{-6} SI units @ 20°C		[85]
Speed of sound:	1203 m/s @ 20°C		[20]
	1174 @ 25°C		[85]
	1158 @ 30.5°C		[20]
	1097 @ 41°C		[20]
Heat of melting:	5.719 kJ/mol		[8]
Heat of vaporization:	29.11 kJ/mol		[8]
Heat of sublimation:	NA		
Heat capacity @ 25°C:	0.1264 kJ/(mol-K)	(liq)	[8]
	0.0753	(gas)	[8]
Heat of combustion:	-1791 kJ/mol @ 25°C	(liq)	[85]
	-1821.38	(gas)	[58]
Heat of formation:	-247.8 kJ/mol @ 25°C	(liq)	[8]
	-216.7	(gas)	[8]
Gibbs (free) energy:	-155.8 kJ/mol @ 25°C	(liq)	[8]
	-153.1	(gas)	[8]

Analytical chemistry: pKa = 24.2 [58]
pKh = -2.85 [58]
pKs = 32.5 [58]

Electrochemical data: [4], [15], [25].

Clay-organic interaction data: 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. Basal spacings of montmorillonite samples containing Na^+, K^+, Ca^{2+} and increasing proportions of 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. [75]

Solubility: Miscible in water, ethanol, ether, benzene, and most oils.

Form: Colorless liquid; fragrant, characteristic mint-like odor; pungent, sweetish taste.

Use: Solvent for fats, oils, waxes, resins, nitrocellulose, cellulose, acetylene and many other substances; chemical manufacturing; dyestuffs; storing acetylene gas; cleaning and drying of precision equipment; purifying paraffin; hardening and dehydrating tissues; specification testing of vulcanized rubber products; paint, varnish and lacquer solvent.

Fire and Explosion Hazard: Very high.
Flash point: -18°C (CC)[63]; -9°C (OC) [58]
lel: 2.6%; uel: 12.8% [63]
Autoign. temp.: 465°C [63]
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_2, dry chemical or alcohol foam. Water should not be used as it will scatter and spread fire.

Incompatible: With chloroform, ($CHCl_3$+a base), CrO, $Cr(OCl_2)$, (nitric+ acetic acid), NOCl, nitrosyl perchlorate, nitryl perchlorate, permonosulfuric acid, potassium tertbutoxide, NaOBr, (sulfuric acid+ potassium dichromate), (thio-diglycol+hydrogen peroxide), H_2O_5S, trichloromelamine, bromoform, HNO_3, activated C, H_2SO_4, BF_3, Br_2, chromyl chloride, H_2O_2, F_2O_2, SCl_2, thiotrithiaxyl perchlorate. Strong oxidizing agents.

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, respirator). Keep container tightly closed. Store in cool, dry, well-ventilated, flammable liquid storage area.

Health effects: 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. Eye irritation. CNS effects. Serious poisonings rare.

Toxicity: Low
TWA: 750 ppm
STEL: 1000 ppm
CL: 3000 ppm
IDLH: 20000 ppm
Peak: 6000 ppm for 30 min duration
Odor threshold: 1-5 mg/m^3 (.5-2 ppm)
Oral:
Non-lethal: 440 $\mu g/m^3$/6 min
10 mg/m^3/6 hr
Lethal dose: 50 mL (estimated)
Inhalation:
Non-lethal: 500 ppm--Eye irritation
12000 ppm--CNS effects

BENZENE C_6H_6 CAS RN: 71432

Syn: Benzol; benzolene; bicarburet of hydrogen; carbon oil; coal naphtha; cyclohexatriene; mineral naphtha; motor benzol; NCI-c55276; phenyl hydride; pyrobenzol; Benzole; Polystream; phene.

Chemical formula: C_6H_6 Monocyclic Aromatic Hydrocarbon

Physical properties:

Relative molecular mass:	78.1134	
Specific gravity:	0.8765	[85]
Boiling point:	80.1°C	[85]
Melting point:	5.5°C	[85]
Refractive index:	1.5011	[85]
Vapor pressure:	10.13 kPa @ 20°C	[52]
Vapor density:	2.77	[63]
Evaporation rate:	5.1	[58]
Relative permittivity:	2.284 @ 20°C	[85]
	2.275 @ 25°C	[85]
	2.073 @ 129°C	[85]
Loss tangent	NA	
Relaxation time:	NA	
Thermal conductivity:	0.146 W/(mol-K) @ 20°C	[20]
	0.141 @ 40°C	[20]
	0.136 @ 60°C	[20]
Electrical resistivity:	0.1316 MOhm-m @ NA	[8]
Critical temperature:	289.01°C	[58]
Critical pressure:	4.898 MPa	[58]
Dynamic viscosity:	0.912 mPa-s @ 0°C	[85]
	0.758 @ 10°C	[85]
	0.652 @ 20°C	[85]
	0.564 @ 30°C	[85]
	0.503 @ 40°C	[85]
	0.442 @ 50°C	[85]
Kinematic viscosity:	1.041 $\mu m^2/s$ @ 0°C	
	0.865 @ 10°C	
	0.744 @ 20°C	
	0.643 @ 30°C	
	0.574 @ 40°C	
	0.504 @ 50°C	
Surface tension:	30.22 mN/m @ 10°C air	[85]
	28.85 @ 20°C air	[85]
	27.56 @ 30°C air	[85]
	26.14 @ 40°C	[10]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.001213 K^{-1}	[58]
Compressibility:	0.864 nPa^{-1} @ 10°C	[85]
	0.937 @ 20°C	[85]
	1.012 @ 30°C	[85]
	1.096 @ 40°C	[85]
Vapor diffusivity:	7.7 $\mu m^2/s$ @ 0°C	[52]

Solution diffusivity:	1.53 nm^2/s in CCl_4		[52]
Electric dipole moment:	0		[8]
Ionization potential:	9.24 eV (S_tPI)		[85]
Volume susceptibility:	-7.68×10^{-6} SI units		[85]
Speed of sound:	1295 m/s @ 25°C		[85]
Heat of melting:	9.872 kJ/mol		[8]
Heat of vaporization:	30.78 kJ/mol		[8]
Heat of sublimation:	44.572 kJ/mol		[58]
Heat capacity @ 25°C:	0.1356 kJ/(mol-K)	(liq)	[85]
	0.0816	(gas)	[85]
Heat of combustion:	-3269 kJ/mol @ 25°C	(liq)	[85]
Heat of formation:	49.03 kJ/mol @ 25°C	(liq)	[8]
	82.98	(gas)	[8]
Gibbs (free) energy:	124.4 kJ/mol @ 25°C	(liq)	[8]
	129.7	(gas)	[8]

Analytical chemistry: pKh = 9.4 [58]

Electrochemical data: [2], [23], [35], [36], [48], [51], [57], [66].

Clay-organic interaction data: Absorption by montmorillonite and vermiculite samples previously dehydrated at 293 K. Intercal-ation by montmorillonite saturated with Cu^{2+}. Increase in basal spacing of montmorillonite and hectorite complexes with a series of alkylammonium ions on intercalation of benzene. Frequencies of C-C stretching and C-H out-of-plane vibrations of benzene in the liquid state and when adsorbed by Cu(II)montmorillonite. [75]

Solubility: Slightly soluble in water; miscible in ethanol, ether, acetone, chloroform, carbon disulfide, carbon tetrachloride, glacial acetic acid, oils and most organic solvents. (0.07g/100g water @ 22°C [8]).

Form: Clear, colorless liquid; characteristic gasoline-like odor.

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; 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.

Fire and Explosion Hazard: Very high.
Flash point: -11°C (CC) [63]
lel: 1.4%; uel: 8.0% [63]
Autoign. temp.: 562°C [63]
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. Fight fire with foam, CO_2 or dry chemical. Water may be ineffective .

Incompatible: With oxidizing materials such as BrF_5, Cl_2, CrO_3, O_2NClO_4, O_2, O_3, perchlorates, ($AlCl_3$+$FClO_4$), (H_2SO_4+permanganates), K_2O_2, ($AgClO_4$-acetic acid), Na_2O_2, boron hydride, sulfuric acid, nitric acid.

Handling: Avoid heat, flame and sources of ignition. Use with adequate ventilation. Respirator required. Self-contained breathing apparatus recommended. Do not allow skin contact (PVA synthetic latex gloves, lab coat, chemical goggles or face shield). 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.

Health effects: Poisoning occurs most commonly through inhalation of the vapor, though benzene can penetrate the skin, and poison in that way. 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 the point of view of causing damage to the blood-forming system, provided the exposure is not repeated. Benzene is a common air contaminant. Listed as a carcinogen by the EPA.

Toxicity: Moderate.
TWA: 10 ppm
STEL: 25 ppm
CL: 25 ppm
IDLH: 2000 ppm
Peak: 50 ppm for 10 min duration
Odor threshold: 1-50 ppm
Exposure: Symptoms of illness begin to occur at concentrations of 500 ppm. Severe toxic effects result after an exposure of 1500 ppm over a 60 min period.
Inhalation:
Non-lethal: 100 ppm/10 yr at int.--Carcinogenic effects
210 ppm--Blood effects
100 ppm--CNS effects
Lethal dose: 20000 ppm/5 min
Toxic conc.: 400 ppm/8 yr at int.--Equivocal tumorigenic effect
2100 mg/m^3/4 yr at int.--Carcinogenic effect
Oral:
Non-lethal: 130 mg/kg--CNS effects

BIS(2-ETHYLHEXYL)PHTHALATE $C_{24}H_{38}O_4$ CAS RN: 117817

Syn: Di(2-ethylhexyl)phthalate; dioctyl phthalate; 1,2-Benzene-dicarboxylic acid bis(2-ethylhexyl) ester; bis(2-ethylhexyl)-1,2-benzenedicarboxylate; di(2-ethylhexyl)ortho-phthalate; di-sec-octyl phthalate; bis(2-ethylhexyl) ester phthalic acid; DOP; DEHP; 2-ethylhexyl phthalate; NCI-c52733; Octoil; phthalic acid.

Chemical formula: $1,2\text{-}C_6H_4[CO_2CH_2CH(C_2H_5)C_4H_9]_2$ Phthalate Ester

Physical properties:

Relative molecular mass:	390.5618	
Specific gravity:	0.9843	[8]
Boiling point:	384°C	[8]
Melting point:	-50°C	[8]
Refractive index:	1.4859	[8]
Vapor pressure:	0.07 mPa @ 183°C	[58]
Vapor density:	13.45	[80]
Evaporation rate:	NA	
Relative permittivity:	5.3 @ 20°C	[8]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	NA	
Electrical resistivity:	NA	
Critical temperature:	NA	
Critical pressure:	NA	
Dynamic viscosity:	381 mPa/s @ 0°C	[58]
	81.4 @ 20°C	[8]
	56.5 @ 25°C	[58]
Kinematic viscosity:	387 $\mu m^2/s$ @ 0°C	
	82.7 @ 20°C	
	57.4 @ 25°C	
Surface tension:	15 mN/m @ 20°C	[86]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.00076 K^{-1}	[58]
Compressibility:	NA	
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	9.473×10^{-30} C-m	[8]
Ionization potential:	NA	
Volume susceptibility:	NA	
Speed of sound:	NA	
Heat of melting:	NA	
Heat of vaporization:	NA	
Heat of sublimation:	NA	
Heat capacity:	NA	
Heat of combustion:	-13747 kJ/mol @ 25°C (liq)	[86]
Heat of formation:	NA	
Gibbs (free) energy:	NA	

Analytical chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Almost insoluble in water; miscible with mineral oil. (0.01g/100g water [8]).

Form: Colorless to light-colored oily liquid; mild odor.

Use: Plasticizer for many resins and elastomers; organic pump fluid; plastics manufacturing and recycling, processing.

Fire and Explosion Hazard: Low.
Flash point: 218°C (OC) [86]
lel: NA
Autoign. temp.: NA
When heated to decomposition it emits an acrid smoke. Fight fire with foam, CO_2 or dry chemical. Water or foam may cause frothing.

Incompatible: Can react with oxidizing materials.

Handling: Use in well ventilated area. Avoid contact with skin or eyes. Store in cool, dry, well-ventilated storage area.

Health effects: Mild eye and skin irritation. Possible liver damage, reproductive effects, embryotoxicity, and teratogenicity; possible carcinogenic potential.

Toxicity: Very low.
TLV: 5 mg/cubic m (0.5 ppm)
Odor threshold: NA
Oral:
Non-lethal: 143 mg/kg-Gastrointestinal tract effects, diarrhea, constipation, ulceration.

BROMOFORM $CHBr_3$ CAS RN: 75252

Syn: Tribromomethane; methenyl tribromide, NCI-c55130.

Chemical formula: CHBr3 Aliphatic Polybrominated Hydrocarbon

Physical properties:

Relative molecular mass:	252.73094	
Specific gravity:	2.8899	[85]
Boiling point:	149.5°C	[85]
Melting point:	8.3°C	[85]
Refractive index:	1.5976	[85]
Vapor pressure:	0.667 kPa @ 20°C	[5]
Vapor density:	8.7	[37]
Evaporation rate:	NA	
Relative permittivity:	4.39 @ 20°C	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	NA	
Electrical resistivity:	>0.5 MOhm-m @ 25°C	[58]
Critical temperature:	NA	
Critical pressure:	NA	
Dynamic viscosity:	2.151 mPa-s @ 15°C	[58]
	1.89 @ 25°C	[85]
	1.741 @ 30°C	[58]
Kinematic viscosity:	0.745 $\mu m^2/s$ @ 15°C	
	0.654 @ 25°C	
	0.602 @ 30°C	
Surface tension:	46.83 mN/m @ 10°C vapor	[8]
(calculated)	45.52 @ 20°C	[8]
	44.22 @ 30°C	[8]
	42.91 @ 40°C	[8]
	41.60 @ 50°C	[8]
	40.29 @ 60°C	[8]
	38.98 @ 70°C	[8]
	37.68 @ 80°C	[8]
	36.37 @ 90°C	[8]
	35.06 @ 100°C	[8]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	NA	
Compressibility:	NA	
Vapor diffusivity:	2.9 $\mu m^2/s$ in Acetone	[52]
	0.53 in i-Amylalcohol	[52]
	1.08 in Ethanol	[52]
	3.62 in Ethyl ether	[52]
	2.20 in Methanol	[52]
	0.94 in n-Propanol	[52]
Solution diffusivity:	NA	
Electric dipole moment:	3.30×10^{-30} C-m	[85]
Ionization potential:	10.51 eV (PI)	[85]
Volume susceptibility:	-11.9×10^{-6} SI units @ 20°C	[85]
Speed of sound:	NA	

Heat of melting:	NA		
Heat of vaporization:	38.91 kJ/mol		[58]
Heat of sublimation:	NA		
Heat capacity @ 17-21°C:	0.13284 kJ/(mol-K)	(liq)	[58]
@ 25°C	0.07101	(gas)	[8]
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)	[58]
	16.736	(gas)	[58]
Gibbs (free) energy:	NA	(liq)	
	7.453 kJ/mol @ 25°C	(gas)	[8]

Analytical chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Slightly soluble in water; soluble in benzene, chloroform, solvent naphtha, fixed and volatile oils; miscible with ethanol, ether. (0.1g/100g water @ 20°C [37]; 0.318% in water @ 30°C [58]; 1 part in 800 in water [88]).

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. 3-4% alcohol added as a preservative in commercial preparations.

Use: As a 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; an 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.

Fire and Explosion Hazard: Very low.
Flash point: not combustible.
lel: not combustible
Autoign. temp.: not combustible
Nonflammable. Dangerous when heated to decomposition as it emits highly toxic fumes of hydrogen bromide and bromine. Can be an explosion hazard, especially when heated.

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

Handling: Keep away from heat and light. Use with adequate ventilation (fume hood). Avoid breathing vapor (respirator). Avoid contact with eyes, skin and clothing (goggles and face shield,neoprene or rubber gloves, lab coat, apron). Keep container tightly closed. Store in secure poison area. Keep out of light.

Health effects: Bromoform is toxic by ingestion, inhalation and skin adsorption. Vapors or fluid can cause irritation of skin, eyes, and mucous membranes. Inhalation of vapors may cause 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 CNS depression and liver damage. Abuse may lead to habituation or addiction.

Toxicity: Moderate.
TWA: 0.5 ppm (skin)
Odor threshold: approx. 500 ppm

CARBON TETRACHLORIDE CCl_4 CAS RN: 56235

Syn: Asordin; Benzinoform; Carbona; carbon chloride; carbon tet; ENT 4705; Freon 10; Katarine; methanetetrachloride; Necatorina; perchloromethane; Phoenipine; Pyrene; Spectral; Tetra; tetrachlorocarbon; tetrachloromethane; Tetracol; Tetraform.

Chemical formula: CCl_4 Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	153.823	
Specific gravity:	1.5940	[85]
Boiling point:	76.638°C	[58]
Melting point:	-22.82°C	[58]
Refractive index:	1.46018	[58]
Vapor pressure:	12.13 kPa @ 20°C	[37]
Vapor density:	5.32	[85]
Evaporation rate:	12.8	[37]
	6.0	[58]
	0.33	[5]
Relative permittivity:	2.238 @ 20°C	[85]
	2.2288 @ 25°C	[58]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.113 W/(m-K) @ -20°C	[20]
	0.109 @ 0°C	[20]
	0.105 @ 20°C	[20]
	0.101 @ 40°C	[20]
	0.9768 @ 50°C	[85]
	0.972 @ 60°C	[20]
Electrical resistivity:	2.5×10^9 MOhm-m @ 18°C	[8]
Critical temperature:	283.4°C	[58]
Critical pressure:	4.516 MPa	[58]
Dynamic viscosity:	1.329 mPa-s @ 0°C	[85]
	1.038 @ 15°C	[85]
	0.969 @ 20°C	[85]
	0.9004 @ 25°C	[58]
	0.843 @ 30°C	[85]
	0.739 @ 40°C	[85]
	0.651 @ 50°C	[85]
	0.585 @ 60°C	[85]
	0.524 @ 70°C	[85]
	0.468 @ 80°C	[85]
	0.426 @ 90°C	[85]
	0.384 @ 100°C	[85]

Kinematic viscosity:	0.834 $\mu m^2/s$	@ 0°C	
	0.651	@ 15°C	
	0.608	@ 20°C	
	0.5649	@ 25°C	
	0.529	@ 30°C	
	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:	29.49 mN/m	@ 0°C	[8]
([8] values are	29.43	@ 10°C	[8]
calculated)	26.95	@ 20°C vapor	[85]
	26.13	@ 25°C	[58]
	25.82	@ 30°C	[8]
	24.59	@ 40°C	[8]
	23.37	@ 50°C	[8]
	22.15	@ 60°C	[8]
	17.26	@ 100°C	[85]
	6.53	@ 200°C	[85]
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	0.001229 K^{-1}		[58]
Compressibility:	0.885 nPa^{-1}	@ 0°C	[85]
	0.945	@ 10°C	[85]
	1.04	@ 20°C	[85]
	1.0799	@ 25°C	[58]
	1.128	@ 30°C	[85]
	1.220	@ 40°C	[85]
	1.320	@ 50°C	[85]
	1.426	@ 60°C	[85]
	1.543	@ 70°C	[85]
Vapor diffusivity:	29.3 $\mu m^2/s$	@ 0°C in H_2	[52]
	6.36	@ 0°C in O_2	[52]
Solution diffusivity:	2.04 nm^2/s	in Benzene	[52]
	1.49	in Cyclohexane	[52]
	0.776	in Decalin	[52]
	1.02	in Dioxane	[52]
	1.5	in ethanol	[52]
	3.17	in n-Heptane	[52]
	0.961	in Kerosene	[52]
	2.30	in Methanol	[52]
	2.57	in i-Octane	[52]
	0.735	in Tetralin	[52]
Electric dipole moment:	0		[58]
Ionization potential:	11.47 eV (PI)		[85]
Volume susceptibility:	-0.691×10^{-6} SI units	@20°C	[85]
Speed of sound:	926 m/s	@ 25°C	[85]
	852	@ 50°C	[20]
Heat of melting:	2.43 kJ/mol		[58]
Heat of vaporization:	29.96 kJ/mol		[58]

Heat of sublimation:	32.62 kJ/mol		[8]
Heat capacity @ 25°C:	0.1327 kJ/(mol-K)	(liq)	[85]
	0.0833	(gas)	[85]
Heat of combustion:	-258.24 kJ/mol @ 25°C	(liq)	[20]
	-290.98	(gas)	[20]
Heat of formation:	-135.44 kJ/mol @ 25°C	(liq)	[58]
	-95.81	(gas)	[58]
Gibbs (free) energy:	-62.68 kJ/mol @ 25°C	(liq)	[8]
	-53.59	(gas)	[8]

Analytical chemistry: Koc = 537 [60]

Electrochemical data: NA

Clay-organic interaction data: Sorption of carbon tetrachloride on soil and clay. [60]

Solubility: Almost insoluble in water; miscible with alcohol, acetone, ether, benzene, chloroform, solvent naphtha, petroleum ether, most fixed and volatile oils. (0.097 per 100 parts water @ 0°C [8]; 0.08 per 100 parts water @ 20°C [8]; 0.08g/100g water @ 20°C [37]; 0.077% in water @ 25°C [58]).

Form: Colorless liquid; sweetish, aromatic, moderately strong ether-like or chloroform-like odor.

Use: In manufacture of fluorocarbons for aerosols, refrigerants and fire extinguishants; as an agricultural grain fumigant and pesticide; in polymer technology as reaction medium, catalyst and chain transfer agent, and solvent for resins; in organic synthesis for chlorination of organic compounds in soap perfumery and insecticide industries; as an 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; as azeotropic drying agent for wet spark plugs in automobiles; as 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.

Fire and Explosion Hazard: Very low.
Flash point: not combustible
lel: not combustible
Autoign. temp.: not combustible
Nonflammable. If heated may decompose forming toxic gases and vapors (phosgene, chlorine gas, hydrogen chloride, carbon monoxide, hydrochloric acid). Severe reaction with allyl alcohol, Al, $Al(C_2H_5)_3$, Ba, (benzoyl peroxide + C_2H_4), Be, BrF_3, $Ca(OCl)_2$, diborane, C_2H_4, dimethyl formamide, disilane, F_2, Li, Mg, liquid O_2, Pu, K, ($AgClO_4$ + HCl), potassium-tert-butoxide, Na, NaK, tetrasilane, trisilane, U, Zr, burning wax. Do not use to put out fires.

Incompatible: Chemically active metals such as sodium, potassium and magnesium; aluminum trichloride, calcium disilicide, chlorine trifluoride, decarborane (14), dibenzoyl peroxide, N-N-dimethylformamide, 1,2,3,4,5,6-hexachlorocyclohexane; dinitrogen teraoxide, fluorine, metals, potassium-tert-butoxide.

Handling: Keep away from heat, flame and sources of ignition. Do not get in eyes, on skin or on clothing (nitrile or PVA synthetic latex gloves, protective suit, chemical safety goggles and face shield). Use with adequate ventilation (fume hood). Do not breath vapors (organic vapor canister respirator with full mask). Keep container tightly closed. Store in secure poison area.

Health effects: Carbon tetrachloride is highly toxic by ingestion, inhalation and skin contact. 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. Eye contact with the liquid causes burning and intense irritation. Delayed effects of short-term exposure include damage to the heart, liver and kidneys. Symptoms of liver damage include yellow jaundice and dark urine. Chronic effects of overexposure may include kidney and/or liver damage and CNS depression. 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.

Toxicity: High.
TWA: 5 ppm
CL: 25 ppm
ANSI TWA: 10 ppm
Peak: 200 ppm for 5 min in a 4 hr period if no other measurable exposure occurs
Odor threshold: 10-50 ppm
Exposure: Concentrations of the order of 1000 to 1500 ppm are sufficient to cause symptoms if exposure continues for several hours. Human fatalities from acute renal damage have occurred after exposure to concentrations of 1000-2000 ppm for about 1/2 to 1 hour. Adverse effects have been reported in workmen who were repeatedly exposed to concentrations between 25 and 30 ppm. No adverse symptoms resulted from repeated exposure to 10 ppm.
Oral:
Non-lethal: 1800 mg/kg--Pulmonary system effects.
1700 mg/kg--CNS effects.
Lethal dose: 43 mg/kg
Inhalation:
Non-lethal: 317 ppm/30 min--Gastrointestinal tract eff.
Lethal dose: 1000 ppm

CHLOROBENZENE C_6H_5Cl CAS RN: 108907

Syn: Benzene chloride; phenyl chloride; chlorbenzene; chlorbenzol; monochlorbenzene; monochlorobenzene; NCI-c54886; MCB.

Chemical formula: C_6H_5Cl Monocyclic Aromatic Hydrocarbon

Physical properties:

Relative molecular mass:	112.5885	
Specific gravity:	1.1058	[85]
Boiling point:	131.687°C	[58]
Melting point:	-45.58°C	[58]
Refractive index:	1.5241	[85]
Vapor pressure:	1.17 kPa @ 20°C	[37]
Vapor density:	3.88	[63]
Evaporation rate:	1.07	[5]
Relative permittivity:	6.30 @ -20°C	[85]
	5.71 @ 20°C	[85]
	5.621 @ 25°C	[85]
	5.552 @ 30°C	[58]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.126 W/(m-K) @ 12°C	[8]
Electrical resistivity:	NA	
Critical temperature:	359.2°C	[8]
Critical pressure:	4.519 MPa	[8]
Dynamic viscosity:	0.900 mPa-s @ 15°C	[85]
	0.799 @ 20°C	[85]
	0.7184 @ 30°C	[58]
	0.631 @ 40°C	[85]
	0.431 @ 80°C	[85]
Kinematic viscosity:	0.814 $\mu m^2/s$ @ 15°C	
	0.723 @ 20°C	
	0.6497 @ 30°C	
	0.571 @ 40°C	
	0.390 @ 80°C	
Surface tension:	33.56 mN/m @ 20°C vapor	[85]
	32.96 @ 20°C	[58]
	31.98 @ 30°C	[58]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.000990 K^{-1}	[58]
Compressibility:	0.738 nPa^{-1} @ 20°C	[85]
	0.784 @ 30°C	[85]
	0.832 @ 40°C	[85]
Vapor diffusivity:	7.5 $\mu m^2/s$ @ 30°C	[8]
Solution diffusivity:	2.66 nm^2/s in Benzene	[8]
Electric dipole moment:	5.637 x 10^{-30} C-m	[8]
Ionization potential:	9.07 eV (PI)	[85]
Volume susceptibility:	-8.65 x 10^{-6} SI units @ 20°C	[85]

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:	9.546	kJ/mol		[8]
Heat of vaporization:	36.55	kJ/mol		[8]
Heat of sublimation:	41.07	kJ/mol		[8]
Heat capacity @ 25°C:	0.146	kJ/(mol-K)	(liq)	[8]
	0.0987		(gas)	[8]
Heat of combustion:	-3088	kJ/mol @ 25°C	(liq)	[20]
	-3130		(gas)	[20]
Heat of formation:	10.80	kJ/mol @ 25°C	(liq)	[8]
	52.3		(gas)	[20]
Gibbs (free) energy:	89.26	kJ/mol @ 25°C	(liq)	[8]
	NA		(gas)	

Analytical chemistry: NA

Electrochemical data: [49], [65], [82].

Clay-organic interaction data: NA

Solubility: Almost insoluble in water; very soluble in benzene; miscible with ethanol, ether, chloroform. (0.05g/100g water @ 20°C [8]).

Form: Clear, colorless liquid; faint, almond-like odor.

Use: Manufacture of phenol, aniline, DDT, picric acid, betachlor-oanthraquinone, rubber adhesives, and adhesives; as an inter-mediate 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.

Fire and Explosion Hazard: High.
Flash point: 28.9°C (CC) [63]
lel: 1.3%; uel: 7.1% [63]
Autoign. temp.: 638°C [63]
Flammable liquid. Dangerous fire hazard when exposed to heat, sparks or flame. Flashback along vapor trail may occur. Also violent reaction with AgClO4, dimethyl sulfoxide. Moderate explosion hazard when exposed to heat or flame. Dangerous as it may emit highly toxic fumes of hydrogen chloride, phosgene, and carbon monoxide. Can react vigorously with oxidizing materials. Fight fire with foam, CO_2 or dry chemicals (water spray to blanket fire). Water may be ineffective.

Incompatible: Strong oxidizers; $AgClO_4$, dimethyl sulfoxide; finely divided Na.

Handling: Keep away from heat, sparks and flame. Avoid breathing vapor. Avoid repeated or prolonged eye or skin contact (neoprene or PVA synthetic latex gloves, lab coat). Use in well-ventilated area (fume hood). Respirator recommended. Keep container tightly closed. Bond and ground containers when transferring liquid. Store in cool, dry, well-ventilated flammable liquid storage area.

Health effects: Chlorobenzene is a fairly strong narcotic and possesses only slight irritant qualities. Short term exposure may cause drowsiness, incoordination, and unconsciousness. It may also cause irritation of the eyes, nose, and skin. Exposures to high levels might also cause liver damage. Prolonged or repeated skin contact may cause skin 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. The urine may be burgundy red, and the red blood cells show degenerative and regenerative changes.

Toxicity: Moderate.
TWA: 75 ppm
IDLH: 2400 ppm
Odor threshold: 0.21-60 ppm
Exposure: Eye and nasal irritation begin to occur at about 200 ppm. Severe toxic effects start at about 400 ppm.

CHLOROETHANE C_2H_5Cl CAS RN: 75003

Syn: Ethylchloride; monochloroethane; chlorethyl; aethylis chloridum; ether chloratus; hydrochloric ether; muriatic ether; Kelene; Chelen; Anodynon; Chloryl Anesthetic; Narcotile.

Chemical formula: CH_3CH_2Cl Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	64.5145		
Specific gravity:	0.8979		[85]
Boiling point:	12.27°C		[58]
Melting point:	-136.4°C		[58]
Refractive index:	1.3676		[85]
Vapor pressure:	141.8 kPa @ 20°C		[37]
Vapor density:	2.22		[88]
Evaporation rate:	>>1		[37]
Relative permittivity:	9.45 @ 20°C		[8]
	6.29 @ 170°C		[20]
Loss tangent:	NA		
Relaxation time:	NA		
Thermal conductivity:	0.009288 W/(m-K)		[58]
Electrical resistivity:	NA		
Critical temperature:	187.2°C		[8]
Critical pressure:	5.269 MPa		[8]
Dynamic viscosity:	0.292 mPa-s @ 5°C		[58]
	0.279 @ 10°C		[58]
	0.278 @ 20°C		[52]
	0.234 @ 40°C		[52]
Kinematic viscosity:	0.325 $\mu m^2/s$ @ 5°C		
	0.311 @ 10°C		
	0.310 @ 20°C		
	0.261 @ 40°C		
Surface tension:	21.18 mN/m @ 5°C		[8]
	20.58 @ 10°C		[8]
	19.5 @ 20°C		[86]
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	0.0021 K^{-1} @ 20°C		[58]
Compressibility:	NA		
Vapor diffusion:	NA		
Solution diffusion:	NA		
Electric dipole moment:	6.838 x 10^{-30} C-m		[8]
Ionization potential:	10.97 eV (EI)		[85]
Volume susceptibility:	NA		
Speed of sound:	NA		
Heat of melting:	4.455 kJ/mol		[8]
Heat of vaporization:	24.67 kJ/mol		[8]
Heat of sublimation:	NA		
Heat capacity @ 25°C:	0.1112 kJ/(mol-K)	(liq)	[30]
	0.0624	(gas)	[30]

Heat of combustion:	-1350	kJ/mol @ 20°C	(liq)	[58]
	-1413		(gas)	[58]
Heat of formation:	-136.52	kJ/mol @ 25°C	(liq)	[58]
	-112.3		(gas)	[8]
Gibbs (free) energy:	-60.54	kJ/mol @ 25°C	(gas)	[8]

Analytical chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Slightly soluble in water; very soluble in ethanol; miscible with ether. (0.57g/100g water @ 20°C [37]; 0.45g/100g water @ 0°C [8]; 48.3g/100ml alcohol [88]).

Form: Colorless liquid; gas at room temperatures and pressures; characteristic pungent, ether-like odor; burning taste.

Use: In production of tetraethyl lead and ethyl cellulose; as a local or general anesthetic; as a refrigeration compound; solvent for fats oils, waxes, phosphorus, acetylene, and many resins; in organic synthesis of perchloroethane, esters, and Grignard reagents; manufacture of dyes, drugs, perfumes; as a propellant in aerosols; insecticides.

Fire and Explosion Hazard: Very high.
Flash point: -50°C (CC)[37]
lel: 3.8%; uel: 15.4% [37]
Autoign. temp.: 519°C [37]
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. 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. Dangerous explosion hazard, in the form of vapor, when exposed to heat or flame. Fight fire with CO_2 or dry chemical, foam and stopping flow of gas.

Incompatible: With chemically active metals such as sodium, potassium, calcium, powdered aluminum, zinc, and magnesium. Can react vigorously with oxidizing materials.

Handling: Keep away from heat, sparks and open flame. Keep container closed, out of sun, and away from heat. Avoid breathing vapor. Respirator required. Use with adequate ventilation (fume hood). Prevent skin contact (neoprene or rubber gloves, lab coat).

Health effects: Short-term exposure to chloroethane may cause drowsiness, unconsciousness, irregular heart beat, and death. It may also cause irritation of the eyes and abdominal cramps. Spilled on the skin, it may cause frostbite. Long-term exposure may cause liver damage.

Toxicity: Very low.
TWA: 1000 ppm
Odor threshold: 27-33 ppm
Exposure: Inhalation of 40,000 ppm causes dizziness, eye irritation, and abdominal cramps, while inhalation of 33,600 ppm (3.36% by volume) causes a toxic effect after 30 seconds, increasing within five minutes to noisy talkativeness followed by incoordination. At 25,000 ppm there is incoordination; 19,000 ppm causes weak analgesia after 12 minutes, and 13,000 ppm causes slight symptoms of inebriation.
External: 4000 ppm--Eye irritation

CHLOROFORM $CHCl_3$ CAS RN: 67663

Syn: Trichloromethane; formyl trichloride; Freon 20; methane trichloride; methenyl trichloride; methyl trichloride; NCI-co2686; trichloroform.

Chemical formula: $CHCl_3$ Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	119.3779	
Specific gravity:	1.4832	[85]
Boiling point:	61.2°C	[8]
Melting point:	-63.5°C	[8]
Refractive index:	1.4459	[85]
Vapor pressure:	21.33 kPa @ 20°C	[88]
Vapor density:	4.12	[63]
Evaporation rate:	11.6	[37]
	10.45	[58]
Relative permittivity:	5.61 @ -20°C	[85]
	4.806 @ 20°C	[85]
	4.639 @ 25°C	[11]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.121 W/(m-K) @ 12°C	[8]
Electrical resistivity:	>0.5 MOhm-m @ 25°C	[8]
Critical temperature:	263.4°C	[8]
Critical pressure:	5.472 MPa	[8]
Dynamic viscosity:	0.855 mPa-s @ -13°C	[85]
	0.700 @ 0°C	[85]
	0.643 @ 8.1°C	[85]
	0.596 @ 15°C	[85]
	0.58 @ 20°C	[85]
	0.5357 @ 25°C	[58]
	0.514 @ 30°C	[85]
Kinematic viscosity:	0.576 $\mu m^2/s$ @ -13°C	
	0.472 @ 0°C	
	0.434 @ 8.1°C	
	0.402 @ 15°C	
	0.391 @ 20°C	
	0.3612 @ 25°C	
	0.347 @ 30°C	
Surface tension:	27.14 mN/m @ 20°C air	[85]
	26.53 @ 25°C	[58]
	25.25 @ 30°C	[58]
	24.53 @ 40°C	[11]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.00126 K^{-1}	[58]
Compressibility:	0.919 nPa^{-1} @ 10°C	[85]
	0.994 @ 20°C	[85]
	1.081 @ 30°C	[85]
	1.179 @ 40°C	[85]
Vapor diffusivity:	9.1 $\mu m^2/s$ @ 0°C	[52]

Solution diffusivity:	2.5 nm^2/s in Benzene			[52]
	1.38 in Ethanol			[52]
Electric dipole moment:	3.369 x 10^{-30} C-m			[8]
Ionization potential:	11.42 eV (PI)			[85]
Volume susceptibility:	-9.30 x 10^{-6} SI units @ 20°C			[85]
Speed of sound:	983 m/s @ 15°C			[81]
	987 @ 25°C			[85]
Heat of melting:	9.546 kJ/mol			[8]
Heat of vaporization:	29.64 kJ/mol			[8]
Heat of sublimation:	31.32 kJ/mol			[8]
Heat capacity @ 25°C:	0.1155 kJ/(mol-K)		(liq)	[85]
	0.0657		(gas)	[85]
Heat of combustion:	-401.96 kJ/mol @ 25°C		(liq)	[58]
Heat of formation:	-132.3 kJ/mol @ 25°C		(liq)	[8]
	-103.0		(gas)	[8]
Gibbs (free) energy:	-71.9 kJ/mol @ 25°C		(liq)	[8]
	-70.17		(gas)	[8]

Analytical chemistry: NA

Electrochemical data: [83].

Clay-organic interaction data: NA

Solubility: Slightly soluble in water; soluble in acetone; miscible in ethanol, ether, benzene, petroleum ether, carbon tetrachloride, carbon disulfide, oils and most organic solvents. (0.82g/100g water @ 20°C [8]).

Form: Heavy, colorless liquid; characteristic ether-like odor; sweet-tasting. Pure chloroform is light sensitive and reagent grade chloroform usually contains 0.75% ethanol as stabilizer.

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, of fluorocarbon resins; general solvent in plastics, dyes, cleaning and dry cleaning industries; in chemical analysis and assays; in standard solutions as preservative and bactericide.

Fire and Explosion Hazard: Very low but dangerous.
Flash point: not combustible
lel: not combustible
Autoign. temp.: not combustible
Practically nonflammable but very volatile. Slight fire hazard if exposed to high heat. When heated to decomposition it emits toxic fumes of hydrogen chloride, chlorine, phosgene and carbon monoxide. In the presence of air and light, it slowly reacts to form toxic phosgene, chlorine and hydrogen chloride gases.

Incompatible: With strong caustics and chemically active metals such as aluminum, lithium, magnesium powder, sodium, or potassium; acetone + a base, alkali, dinitrogen tetraoxide, fluorine, potassium tert-butoxide, sodium, sodium hydroxide + methanol, potassium hydroxide + methanol, sodium methoxide, triisoprylphosphine, disilane, perchloric acid + phosphorus pentaoxide, sodium methylate, sodium hydroxide.

Handling: Avoid heat and light. Very volatile so use in well ventilated area with a respirator. Prevent skin contact (PVA synthetic latex, neoprene, leather or nitrile gloves, chemical glasses, lab coat). Keep container tightly closed. Store in secure poison area away from light and heat.

Health effects: Inhalation of chloroform causes dilation of the pupils with reduced reaction to light, as well as reduced intraocular pressure. This material is well known as an anesthetic. 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. Listed as a carcinogen by the EPA.

Toxicity: Moderate.
TWA: 10 ppm
CL: 50 ppm
IDLH: 1000
Odor threshold: 50-300 ppm
Exposure: 68,000-82,000 ppm kill most animals in a few minutes. 14,000 ppm is dangerous to life after an exposure of from 30 to 60 minutes. 5000-6000 ppm can be tolerated by animals for 1 hr without serious disturbances. The maximum concentration tolerated for several hours or for prolonged exposure with slight symptoms is 2000-2500 ppm. Inhalation exposure to concentrations >1000 ppm can produce drowsiness, nausea and headache. Chronic exposure to 100-200 ppm has been reported to produce enlarged livers.
Inhalation:
Non-lethal: 1000 mg/m^3/1 yr--Liver and kidney damage
5000 mg/m^3/7 min--CNS effects
Oral:
Lethal dose: 140 mg/kg

CYCLOHEXANE C_6H_{12} CAS RN: 110827

Syn: Benzene hexahydride; hexahydrobenzene; hexamethylene; hexanaphthene.

Chemical formula: $(CH_2)_6$ Saturated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	84.16128	
Specific gravity:	0.77855	[85]
Boiling point:	80.74°C	[85]
Melting point:	6.55°C	[85]
Refractive index:	1.42662	[85]
Vapor pressure:	12.7 kPa @ 20°C	[37]
Vapor density:	2.98	[37]
Evaporation rate:	2.6	[5]
Relative permittivity:	2.023 @ 20°C	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	NA	
Electrical resistivity:	1.43 x 10^9 MOhm-m @ 25°C	[58]
Critical temperature:	280.49°C	[58]
Critical pressure:	4.075 MPa	[58]
Dynamic viscosity:	1.02 mPa-s @ 17°C	[85]
	0.975 @ 20°C	[58]
	0.898 @ 25°C	[58]
	0.820 @ 30°C	[58]
Kinematic viscosity:	1.31 $\mu m^2/s$ @ 17°C	
	1.25 @ 20°C	
	1.15 @ 25°C	
	1.05 @ 30°C	
Surface tension:	26.432 mN/m @ 10°C	[8]
([8] values are calculated)	25.24 @ 20°C	[58]
	24.65 @ 25°C	[58]
	23.74 @ 30°C	[58]
	22.868 @ 40°C	[8]
	21.680 @ 50°C	[8]
	20.492 @ 60°C	[8]
	19.304 @ 70°C	[8]
	18.116 @ 80°C	[8]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.001220 K^{-1}	[58]
Compressibility:	0.988 nPa^{-1} @ 10°C	[85]
	1.110 @ 25°C	[85]
	1.202 @ 35°C	[85]
	1.256 @ 40°C	[85]
	1.314 @ 45°C	[85]
	1.435 @ 55°C	[85]
	1.488 @ 60°C	[85]
	1.784 @ 75°C	[85]

Vapor diffusivity:	8.6 $\mu m^2/s$ @ 45°C in air			[52]
	7.4 @ 15°C in O_2			[52]
	7.6 @ 15°C in N_2			[52]
	31.9 @ 15°C in H_2			[52]
Solution diffusivity:	NA			
Electric dipole moment:	0			[8]
Ionization potential:	9.8 eV (PI,PE)			[85]
Volume susceptibility:	-7.879×10^{-6} SI units @20°C			[85]
Speed of sound:	NA			
Heat of melting:	2.6796 kJ/mol			[8]
Heat of vaporization:	29.977 kJ/mol			[8]
Heat of sublimation:	33.059 kJ/mol			[8]
Heat capacity @ 25°C:	0.1524 kJ/(mol-K)		(liq)	[85]
	0.1063		(gas)	[85]
Heat of combustion:	-3922.5 kJ/mol @ 25°C		(liq)	[85]
Heat of formation:	-156.34 kJ/mol @ 25°C		(liq)	[8]
	-123.22		(gas)	[8]
Gibbs (free) energy:	26.67 kJ/mol @ 25°C		(liq)	[8]
	31.78		(gas)	[8]

Analytical chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Almost insoluble in water; miscible with alcohol, ether, acetone, benzene, carbon tetrachloride, chlorinated hydrocarbons, most other organic solvents. (0.01% in water @ 20°C [58]; <0.01g/100g water @ 20°C [37]; 57g/100mL methanol @ 20°C [88])

Form: Colorless, mobile liquid; mild, sweet odor resembling benzene, chloroform or gasoline.

Use: As a 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 for production of Nylon 66 and engineering plastics; during synthesis of caprolactam in Nylon 66 production; 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; in the industrial recrystallization of steroids.

Fire and Explosion Hazard: Very high.
Flash point: -20°C (CC) [86]
lel: 1.33%; uel: 8.35% [86]
Autoign. temp.: 270°C [86]
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 N_2O_4. Can react vigorously with oxidizing materials. Fire may release toxic gases and vapors (such as carbon monoxide). Fight fire with foam, CO_2 or dry chemical. Water may be ineffective.

Incompatible: Strong oxidizing agents; NsO_4.

Handling: Keep away from heat, sparks and flame. Use with adequate ventilation (fume hood). Avoid breathing vapor (hydrocarbon vapor canister respirator or supplied-air or hose mask). Avoid contact with eyes, skin and clothing (polyethylene, PVC coated nylon, nitrile or neoprene gloves and apron, lab coat, chemical safety goggles or face shield). Keep container tightly closed. Bond and ground container when transferring liquid. Store in cool, dry, well-ventilated flammable liquid storage area.

Health effects: Cyclohexane is moderately toxic if inhaled, swallowed or comes into contact with the eyes or skin. It is a local irritant and CNS depressant. 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.

Toxicity: Moderate.
TWA: 300 ppm
STEL: 375 ppm
IDLH: 10000 ppm
Odor threshold: 0.41-300 ppm
Exposure: Concentration of 5 ppm may cause eye irritation. Prolonged or repeated exposure to concentrations above 300 ppm produces mild irritation of the eyes and upper respiratory tract. Exposure to concentrations above 12000 ppm may have a depressant effect.
Oral:
Lethal dose: 0.5-5 g/kg
60-70 g/L

DI-n-BUTYL PHTHALATE $C_{16}H_{22}O_4$ CAS RN: 84742

Syn: Dibutyl phthalate; DBP; n-butyl phthalate; 1,2-Benzene-dicarboxylic acid dibutyl ester; dibutyl ester phthalic acid; o-bezenedicarboxylic acid dibutyl ester; benzene-o-dicarboxylic acid di-n-butyl ester; dibutyl 1,2-benzenedicarboxylate; RC plasticizer DBP; Witicizer 300.

Chemical formula: $1,2\text{-}C_6H_4(COOC_4H_9)_2$ Phthalate Ester

Physical properties:

Relative molecular mass:	278.3474	
Specific gravity:	1.047 (20/20)	[85]
Boiling point:	340°C	[85]
Melting point:	-35°C	[58]
Refractive index:	1.4911	[85]
Vapor pressure:	<0.0013 kPa @ 20°C	[37]
Vapor density:	9.58	[63]
Evaporation rate:	Almost zero	[37]
Relative permittivity:	6.436 @ 20°C	[8]
	6.436 @ 30°C	[58]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	NA	
Electrical resistivity:	NA	
Critical temperature:	500°C	[86]
Critical pressure:	1.7 MPa	[86]
Dynamic viscosity:	20.3 mPa-s @ 20°C	[24]
	15.4 @ 25°C	[58]
	2.2 @ 100°C	[58]
Kinematic viscosity:	19.39 $\mu m^2/s$ @ 20°C	
	14.7 @ 25°C	
	2.1 @ 100°C	
Surface tension:	33.47 mN/m @ 20°C	[8]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.00086 K^{-1}	[58]
Compressibility:	NA	
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	8.055 x 10^{-30} C-m	[8]
Ionization potential:	NA	
Volume susceptibility:	NA	
Speed of sound:	NA	
Heat of melting:	NA	
Heat of vaporization:	79.2 kJ/mol	[58]
Heat of sublimation:	91.69 kJ/mol	[8]
Heat capacity @ 21°C:	0.498 kJ/(mol-K)	[58]
Heat of combustion:	-8611 kJ/mol (liq)	[58]
Heat of formation:	-841.5 kJ/mol @ 25°C (sol)	[8]
Gibbs (free) energy:	NA	

Analytical chemistry: pKs = 4.2 x 10^{-6} [58]

Electrochemical data: [61].

Clay-organic interaction data: NA

Solubility: Slightly soluble in water; very soluble in ethanol, ether, acetone, benzene. (0.45g/100g water @ 20°C [37]).

Form: Colorless, oily liquid; very weak, aromatic odor.

Use: Liberation 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; use in spray application of nitrocellulose lacquer surface coatings; insect repellent.

Fire and Explosion Hazard: Low.
Flash point: 157°C (CC); 179°C (OC) [86]
lel: 0.5%; uel: 2.5% [86]
Autoign. temp.: 403°C [86]
Slight fire hazard when exposed to heat, flame, or incompatible substances. Violent reaction with chlorine. Fire may emit toxic gases and vapors (such as carbon monoxide and carbon dioxide). Fight fire with CO_2, dry chemical or foam. Water or foam may cause frothing.

Incompatible: Nitrates, strong oxidizers, strong bases and strong acids; chlorine.

Handling: Avoid heat, flame and other sources of ignition. Use in well ventilated area. Avoid skin contact (nitrile, PVA synthetic latex or neoprene gloves, lab coat, chemical goggles or face shield). Respirator recommended to avoid breathing vapors. Store in cool, dry, well-ventilated area.

Health effects: Swallowing di-n-butyl phthalate may cause nausea, dizziness, light sensitivity, and watering and redness of the eyes. Overexposure to hot vapors or mists may cause nose and throat irritation, and produce 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.

Toxicity: Low.
TWA: 5 mg/m^3 (0.5 ppm)
Odor threshold: No data

1,1-DICHLOROETHANE $C_2H_4Cl_2$ CAS RN:75343

Syn: Ethylidene chloride; dichloroethane; asymmetrical dichloroethane; ethylidene dichloride; chlorinated hydrochloric ether.

Chemical formula: CH_3CHCl_2 Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	98.9596		
Specific gravity:	1.1757		[85]
Boiling point:	57.30°C		[58]
Melting point:	-96.96°C		[58]
Refractive index:	1.4164		[85]
Vapor pressure:	24.26 kPa @ 20°C		[37]
Vapor density:	3.42		[80]
Evaporation rate:	11.6		[37]
Relative permittivity:	10.0 @ 18°C		[8]
Loss tangent:	NA		
Relaxation time:	NA		
Thermal conductivity:	NA		
Electrical resistivity:	>0.5882 MOhm-m @ 25°C		[8]
Critical temperature:	250°C		[8]
Critical pressure:	5.066 MPa		[8]
Dynamic viscosity:	0.44 mPa-s @ 20°C		[52]
	0.505 @ 25°C		[58]
	0.430 @ 30°C		[58]
	0.36 @ 40°C		[52]
Kinematic viscosity:	0.37 $\mu m^2/s$ @ 20°C		
	0.430 @ 25°C		
	0.366 @ 30°C		
	0.31 @ 40°C		
Surface tension:	24.75 mN/m @ 20°C		[58]
	23.62 @ 30°C		[58]
	23.4 @ 35°C air		[20]
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	NA		
Compressibility:	NA		
Vapor diffusivity:	NA		
Solution diffusivity:	NA		
Electric dipole moment:	6.87 x 10^{-30} C-m		[8]
Ionization potential:	NA		
Volume susceptibility:	NA		
Speed of sound:	NA		
Heat of melting:	7.875 kJ/mol		[8]
Heat of vaporization:	29.18 kJ/mol		[8]
Heat of sublimation:	30.81 kJ/mol		[8]
Heat capacity @ 25°C:	0.1264 kJ/(mol-k)	(liq)	[8]
	0.0764	(gas)	[8]
Heat of combustion:	-1098 kJ/mol @ 25°C	(liq)	[86]
Heat of formation:	-160.4 kJ/mol @ 25°C	(liq)	[8]
	-130.2	(gas)	[8]

Gibbs (free) energy:	-75.78	kJ/mol @ 25°C	(liq)	[8]
	-73.35		(gas)	[8]

Analytical chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Slightly soluble in water; soluble in acetone, benzene; very soluble in ethanol, ether.(0.5g/100g water @ 30°C [8]).

Form: Colorless, oily liquid; odor and taste as of chloroform.

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 floatation.

Fire and Explosion Hazard: Very high.
Flash point: -5.6°C (CC); 13.9°C (OC) [86]
lel: 5.6%; uel: 11.4% [86]
Autoign. temp.: 458°C [86]
Extremely flammable liquid. Dangerous fire hazard and moderate explosion hazard when exposed to heat or flame. When heated to decomposition it emits very toxic fumes of hydrogen chloride, vinyl chloride, phosgene, and carbon monoxide. Fight fire with alcohol foam, CO_2 or dry chemical. Water may be ineffective.

Incompatible: With strong oxidizers (may cause fire and explosion); with strong caustics (formation of flammable and toxic acetaldehyde gas). Will attack some forms of plastics, rubber, and coatings.

Handling: Avoid heat, flame and sources of ignition. Avoid repeated or prolonged skin contact (PVA synthetic latex or nitrile gloves, chemical goggles, lab coat). Respirator recommended. 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

Health effects: 1,1-Dichloroethane is not known to be an eye irritant. There have been no reported cases of human overexposure by inhalation. 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. 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. Possible embryotoxicity.

Toxicity: Very low.
TWA: 200 ppm
STEL: 250 ppm
OSHA TWA: 100 ppm
Odor threshold: 120-200 ppm

1,2-DICHLOROETHANE $C_2H_4Cl_2$ CAS RN: 107062

Syn: Ethylene dichloride; sym-dichloroethane; ethylene chloride; EDC; glycol dichloride; ethenedichloride; 1,2-bichloridiethane; Dutch liquid; Brocide.

Chemical formula: $ClCH_2CH_2Cl$

Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	98.9596	
Specific gravity:	1.253	[8]
Boiling point:	83.483°C	[58]
Melting point:	-35.66°C	[58]
Refractive index:	1.4448	[85]
Vapor pressure:	8.13 kPa @ 20°C	[80]
Vapor density:	3.35	[41]
Evaporation rate:	4.46	[58]
	0.27	[5]
Relative permittivity:	10.36 @ 25°C	[8]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.126 W/(m-K) @ 20°C	[85]
Electrical resistivity:	0.333 MOhm-m @ 25°C	[8]
Critical temperature:	288.4°C	[52]
Critical pressure:	5.370 MPa	[52]
Dynamic viscosity:	1.077 mPa-s @ 0°C	[85]
	0.887 @ 15°C	[58]
	0.800 @ 19.4°C	[85]
	0.730 @ 30°C	[58]
	0.652 @ 40°C	[85]
	0.565 @ 50°C	[85]
	0.479 @ 70°C	[85]
Kinematic viscosity:	0.860 $\mu m^2/s$ @ 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]
	32.48 @ 20°C	[11]
	31.06 @ 30°C	[11]
	28.27 @ 40°C	[11]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.001141 K^{-1} @ 20°C	[58]
	0.00121 @ 55°C	[58]
Compressibility:	0.742 nPa^{-1} @ 10°C	[85]
	0.797 @ 20°C	[85]
	0.858 @ 30°C	[85]
	0.925 @ 40°C	[85]
Vapor diffusivity:	NA	

Solution diffusivity:	2.8 nm^2/s in Benzene			[52]
Electric dipole moment:	4.003 x 10^{-30} C-m			[8]
Ionization potential:	11.12 eV (PI)			[85]
Volume susceptibility:	-9.51 x 10^{-6} SI units @ 20°C			[85]
Speed of sound:	NA			
Heat of melting:	8.843 kJ/mol			[8]
Heat of vaporization:	32.03 kJ/mol			[8]
Heat of sublimation:	35.46 kJ/mol			[8]
Heat capacity @ 25°C:	0.1294 kJ/(mol-K)		(liq)	[8]
	0.0787		(gas)	[8]
Heat of combustion:	-1111.48 kJ/mol @ 25°C		(liq)	[58]
	-1135		(gas)	[85]
Heat of formation:	-165.3 kJ/mol @ 25°C		(liq)	[8]
	-129.8		(gas)	[8]
Gibbs (free) energy:	-79.68 kJ/mol @ 25°C		(liq)	[8]
	-73.90		(gas)	[8]

Analytical chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Slightly soluble in water; soluble in acetone, benzene; very soluble in ethanol; miscible with ether, chloroform, mineral oil. (0.869g/100g water @ 20°C [80]; 0.92g/100g water @ 30°C [80]).

Form: Heavy, colorless liquid; sweet chloroform-like odor; sweet taste.

Use: Solvent for fats, oils, waxes, gums, resins, and particularly for rubber; manufacture of acetyl cellulose, tobacco extract, etc.; fumigant; degreasers; soaps and scouring compounds; additive in antiknock gasoline; paint and finish removers; in production of vinyl chloride and other halogenated hydrocarbons; lead scavenger; ore flotation. 17th highest volume chemical produced in U.S. (1979).

Fire and Explosion Hazard: High.
Flash point: 12.8°C (CC), 15.8°C (OC) [86]
lel: 6.2%; uel: 15.6% [86]
Autoign. temp.: 413°C [86]
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. Fight fire with foam, CO_2 or dry chemical. Water may be ineffective.

Incompatible: With dinitrogen tetraoxide, metals, strong oxidizing materials.

Handling: Keep away from heat, sparks and flame. Avoid breathing vapor. Use in well-ventilated area (fume hood) with respirator. Avoid skin contact (PVA synthetic latex or nitrile gloves, lab coat, chemical goggles or face shield). Keep container tightly closed. Bond and ground containers when transferring liquid. Store in cool, dry, well-ventilated flammable liquid storage area.

Health effects: In high concentrations, 1,2-Dichloroethane vapors produce irritation of the eyes, skin and respiratory tract. It may also cause drowsiness, headache and vomiting, 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.

Toxicity: Moderate
TWA: 10 ppm
CL: 100 ppm
IDLH: 1000 ppm
Odor threshold: 3-100 ppm
Exposure: Symptoms of illness begin to occur at 100 ppm, and severe toxic effects at 500 ppm (2050 mg/m^3) over a 60 min period.
Inhalation:
Short term limits: 200 ppm for 5 min during any 3 hr period.

1,1-DICHLOROETHENE $C_2H_2Cl_2$ CAS RN: 75354

Syn: Vinylidene chloride; 1,1-dichloroethylene; 1,1-DCE; NCI-c54262; asym-dichloroethylene; VC.

Chemical formula: $CH_2=CCl_2$ Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	96.9438		
Specific gravity:	1.2129		[88]
Boiling point:	31.56°C		[58]
Melting point:	-122.56°C		[58]
Refractive index:	1.4249		[85]
Vapor pressure:	66.67 kPa @ 20°C		[80]
Vapor density:	3.25		[80]
Evaporation rate:	NA		
Relative permittivity:	4.67 @ 16°C		[85]
Loss tangent:	NA		
Relaxation time:	NA		
Thermal conductivity:	NA		
Electrical resistivity:	NA		
Critical temperature:	222°C		[58]
Critical pressure:	5.20 MPa		[58]
Dynamic viscosity:	0.422 mPa-s @ 0°C		[58]
	0.358 @ 20°C		[58]
Kinematic viscosity:	0.348 $\mu m^2/s$ @ 0°C		
	0.295 @ 20°C		
Surface tension:	24 mN/m @ 15°C		[86]
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	NA		
Compressibility:	NA		
Vapor diffusivity:	NA		
Solution diffusivity:	NA		
Electric dipole moment:	4.336×10^{-30} C-m		[8]
Ionization potential:	NA		
Volume susceptibility:	-7.98×10^{-6} SI units @ 15°C		[85]
Speed of sound:	NA		
Heat of melting:	6.519 kJ/mol		[8]
Heat of vaporization:	26.209 kJ/mol		[8]
Heat of sublimation:	34.87 kJ/mol		[8]
Heat capacity @ 25°C:	0.113 kJ/(mol-K)	(liq)	[85]
	0.0673	(gas)	[85]
Heat of combustion:	-1095.95 kJ/mol @ 25°C	(liq)	[58]
Heat of formation:	-24.28 kJ/mol @ 25°C	(liq)	[8]
	1.256	(gas)	[8]
Heat of polymerization:	-75.3 kJ/mol @ 25°C		[58]
Gibbs (free) energy:	24.49 kJ/mol @ 25°C	(liq)	[8]
	24.20	(gas)	[8]

Analytical chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Practically insoluble in water; soluble in ethanol, acetone, benzene and other organic solvents; very soluble in ether. (0.021g/100g water [8]).

Form: Colorless liquid; mild, sweet odor resembling that of chloroform. Commercially contains 0.02% of monomethylether of hydroquinone as inhibitor.

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.

Fire and Explosion Hazard: Very high.
Flash point: -18°C (OC) [86]
lel: 7.3%; uel: 16.0% [86]
Autoign. temp.: 513-555°C [86]
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. Also can explode spontaneously. Reacts violently with chlorosulfonic acid, HNO_3, oleum. Emits highly toxic fumes of hydrogen chloride and phosgene. Can react vigorously with oxidizing materials. At temperatures above 0°C and especially in the presence of sunlight, air, copper and aluminum, polymerizes to a plastic. 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 foam, CO_2 or dry chemical. Water may be ineffective.

Incompatible: With oxidizing materials, air, chlorotrifluoro-ethylene, ozone, perchloryl fluoride, chlorosulfonic acid, HNO_3, oleum.

Handling: Do not expose to air, heat or flame. Avoid breathing vapors. Use with adequate ventilation (fume hood). Respirator required. Prevent skin contact (rubber gloves and boots, goggles or face shield, lab coat). Keep container tightly closed. Bond and ground containers when transferring liquid. Store in cool, dry, well- ventilated flammable liquid storage area.

Health effects: 1,1-Dichloroethene is an irritant to eyes, skin, and mucous membranes. Narcotic in high concentrations. Chronic effects to overexposure may include liver and/or kidney damage, and cardiovascular effects. Moderate carcinogenic potential.

Toxicity: High.
TWA: 1 ppm;
CL: 5 ppm over any 15 minute period
Odor threshold: 500 ppm
Exposure: Irritating to skin after contact of a few minutes.
Inhalation:
Non-lethal: 25 ppm--Liver and kidney damage

TRANS-1,2-DICHLOROETHENE $C_2H_2Cl_2$ CAS RN: 156605

Syn: Acetylene dichloride; trans-acetylene dichloride; 1,2-dichloroethene; 1,2-dichloroethylene; dichloroethylene; sym-dichloroethylene; (E)-1,2-dichloroethene; Dioform.

Chemical formula: ClCH=CHCl Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	96.9438		
Specific gravity:	1.2565		[85]
Boiling point:	47.67°C		[58]
Melting point:	-49.8°C		[58]
Refractive index:	1.4462		[58]
Vapor pressure:	35.33 kPa @ 20°C		[37]
Vapor density:	3.34		[37]
Evaporation rate:	NA		
Relative permittivity:	2.14 @ 25°C		[85]
Loss tangent:	NA		
Relaxation time:	NA		
Thermal conductivity:	NA		
Electrical resistivity:	NA		
Critical temperature:	243.3°C		[8]
Critical pressure:	5.522 MPa		[8]
Dynamic viscosity:	0.423 mPa-s @ 15°C		[58]
	0.404 @ 20°C		[58]
Kinematic viscosity:	0.367 $\mu m^2/s$ @ 20°C		
	0.322 @ 20°C		
Surface tension:	25 mN/m @ 20°C		[8]
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	0.00136 K^{-1}		[58]
Compressibility:	1.119 nPa^{-1} @ 25°C		[85]
Vapor diffusivity:	NA		
Solution diffusivity:	NA		
Electric dipole moment:	2.335 x 10^{-30} C-m		[8]
Ionization potential:	9.64 eV (PI)		[85]
Speed of sound:	NA		
Volume susceptibility:	-8.02 x 10^{-6} SI units @ 15°C		[85]
Heat of melting:	7.201 kJ/mol		[8]
Heat of vaporization:	27.84 kJ/mol		[8]
Heat of sublimation:	28.97 kJ/mol		[8]
Heat capacity @ 25°C:	0.1275 kJ/(mol-K)	(liq)	[30]
	0.0667	(gas)	[8]
Heat of combustion:	-1092.28 kJ/mol @ 18°C	(liq)	[58]
Heat of formation:	-23.14 kJ/mol @ 25°C	(liq)	[58]
	6.157	(gas)	[58]
Gibbs (free) energy:	NA	(liq)	
	26.59 kJ/mol @ 25°C	(gas)	[8]

Analytical chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Slightly soluble in water; very soluble in benzene; miscible in ethanol, ether, acetone, and most organic solvents. (0.35g/100g water [8]; 0.06g/100g water @ 20°C [10]).

Form: Colorless, liquid; slightly acrid, ether-like odor; gradually decomposed by air, light and moisture, forming HCl.

Use: Solvent for fats, phenol, camphor, gums, waxes, oils, lacquers, resins, thermoplastics, and artificial fibers; retarding fermentation; rubber and dye extraction; organic synthesis for polymers and telomers; low temperature solvent for heat-sensitive substances in extraction of caffeine, perfume oils, and fats from flesh of animals; liquid dry cleaning agent; cleaning solution for printed circuit boards; food packaging adhesives; germicidal fumigants.

Fire and Explosion Hazard: High.
Flash point: 2.2°C to 3.9°C (CC) [37]
lel: 9.7%; uel: 12.8% [37]
Autoign. temp.: 460°C [37]
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 flame. Noticeably subject to air oxidation. Contact with strong oxidizers can cause fires and explosions. Fire may release toxic gases such as hydrogen chloride, phosgene, and carbon monoxide. Fight fire with dry chemical, foam or CO_2. Water may be ineffective.

Incompatible: With strong oxidizers, alkalis, difluoromethylene dihypofluorite, nitrogen tetraoxide. Will attack some forms of plastics, rubber, and coatings.

Handling: Avoid heat, sparks or flame. Use with adequate ventilation (fume hood). Respirator recommended. Avoid repeated or prolonged skin contact (rubber gloves, lab coat, splash-proof goggles). Keep container tightly closed. Bond and ground containers when transferring liquid. Store in cool, dry, well-ventilated flammable liquid storage area.

Health effects: Minimal. Trans-1,2-Dichloroethene can affect the body if inhaled, swallowed, eye or skin contact. It is an eye irritant at high concentrations. Overexposure may cause drowsiness, dizziness, and unconsciousness. High concentrations are narcotic and mucous membrane irritant.

Toxicity: Very low.
TWA: 200 ppm
IDLH: 4000 ppm
STEL: 250 ppm
Odor threshold: 0.1 ppm

DIMETHYL SULFOXIDE C_2H_6OS CAS RN: 67685

Syn: Dimethyl sulphoxide; Deltan; Demasorb; Demavet; Demeso; Dermasorb; DMSO; DMS-70; DMS-90; Dolicur; Domosol; Dromisol; Gamasol 90; Hyadur; Infiltrina; methyl sulfoxide; Rimso-50; Somipront; SQ 9453; sulfinylbis[methane]; Syntexan; Topsym (rescinded).

Chemical formula: CH_3SOCH_3 Oxo-sulphur Hydrocarbon

Physical properties:

Relative molecular mass:	78.12904		
Specific gravity:	1.10041		[58]
Boiling point:	189.0°C		[58]
Melting point:	18.54°C		[58]
Refractive index:	1.47933		[58]
Vapor pressure:	0.0493 kPa @ 20°C		[63]
Vapor density:	NA		
Evaporation rate:	NA		
Relative permittivity:	48.9 @ 20°C		[24]
	46.45 @ 25°C		[58]
Loss tangent:	NA		
Relaxation time:	NA		
Thermal conductivity:	NA		
Electrical resistivity:	5 MOhm-m @ 25°C		[58]
Critical temperature:	NA		
Critical pressure:	NA		
Dynamic viscosity:	2.2159 mPa-s @ 20°C		[58]
	1.991 @ 25°C		[58]
	1.654 @ 30°C		[58]
Kinematic viscosity:	2.0137 $\mu m^2/s$ @ 20°C		
	1.809 @ 25°C		
	1.503 @ 30°C		
Surface tension:	NA		
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	0.000928 K^{-1}		[58]
Compressibility:	0.52 nPa^{-1} @ 25°C		[58]
Vapor diffusivity:	NA		
Solution diffusivity:	NA		
Electric dipole moment:	13.54 x 10^{-30} C-m		[58]
Ionization potential:	NA		
Volume susceptibility:	NA		
Speed of sound:	NA		
Heat of melting:	14.368 kJ/mol		[58]
Heat of vaporization:	43.14 kJ/mol		[58]
Heat of sublimation:	77.0 kJ/mol		[58]
Heat capacity @ 25°C:	0.15318 kJ/(mol-K)	(liq)	[58]
Heat of combustion:	-1979 kJ/mol @ 25°C	(liq)	[86]
Heat of formation:	-203.89 kJ/mol @ 25°C	(liq)	[58]
	-151.01	(gas)	[58]
Heat of solution:	18 kJ/mol @ 25°C		[86]
Gibbs (free) energy:	-99.23 kJ/mol @ 25°C	(liq)	[8]

Analytical chemistry: pKa = 1.4 in acetic acid anhydride [58]
-1.54 @ 25°C in aq H_2SO_4 [58]
pKs = 31.8 @ 25°C [58]
17.3 @ 25°C [8]

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Soluble in water, ethanol, ether, acetone, benzene, chloroform. Dissolves some hydrocarbons more than others. Extremely powerful aprotic solvent. (25.3% in water @ 25°C [58]).

Form: Colorless, hygroscopic liquid; practically no odor; slightly bitter taste with sweet after-taste.

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.

Fire and Explosion Hazard: Low.
Flash point: 95°C (OC) [63]; 87.8°C (CC) [86]
lel: 2.6%; uel: 28.5% [63]
Autoign. temp.: 215°C [63]
Combustible liquid. Low fire hazard when exposed to heat or flame. When heated to decomposition it emits toxic fumes (sulfur dioxide, formaldehyde, methyl mercaptan). Can react with oxidizing materials. Reacts violently with many acyl and aryl halides, bromobenzyl acetanilide, cyanuric chloride, IF_2, magnesium perchlorate, CH_3Br, NIO_4, P_2O_3, AgF, NaH. Fight fire with water, foam, alcohol foam, dry chemical or CO_2.

Incompatible: Strong oxidizing agents; acyl halides; boron compounds; N_2O_4; iodine pentafluoride; magnesium perchlorate; metal oxosalts; non-metal halides; perchloric acid; periodic acid; silver difluoride; sodium hydride; sulfur trioxide.

Handling: Avoid heat or flame. Use with adequate ventilation. Avoid breathing vapors (respirator if airborne spray or droplets present). Avoid skin or eye contact (neoprene, natural rubber or latex gloves, chemical safety goggles, lab coat).

Health effects: DMSO is harmful if ingested. 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. It is an experimental teratogen.

Toxicity: Low.
TWA: NA
Odor threshold: Practically no odor.

1,4-DIOXANE $C_4H_8O_2$ CAS RN: 123911

Syn: Diethylene dioxide; 1,4-diethylene dioxide; diethylene ether; di(ethylene oxide); 1,4-dioxacyclohexane; dioxan; dioxyethylene ether; glycol ethylene ether; NCI-c03689; p-dioxane; tetrahydrop-dioxin; tetrahydro-1,4-dioxin.

Chemical formula: $O=(CH_2)_4=O$ Epoxide

Physical properties:

Relative molecular mass:	88.1063		
Specific gravity:	1.0337		[85]
Boiling point:	101.32°C		[58]
Melting point:	11.80°C		[58]
Refractive index:	1.4224		[85]
Vapor pressure:	3.87 kPa @ 20°C		[37]
Vapor density:	3.03		[63]
Evaporation rate:	2.42		[58]
Relative permittivity:	2.209 @ 25°C		[85]
Loss tangent:	NA		
Relaxation time:	NA		
Thermal conductivity:	NA		
Electrical resistivity:	NA		
Critical temperature:	312oC		[88]
Critical pressure:	5.137 MPa		[88]
Dynamic viscosity:	1.439 mPa-s @ 15°C		[8]
	1.20 @ 25°C		[88]
	1.087 @ 30°C		[58]
Kinematic viscosity:	1.392 $\mu m^2/s$ @ 15°C		
	1.16 @ 25°C		
	1.052 @ 30°C		
Surface tension:	36.23 mN/m @ 0°C		[8]
(calculated)	34.84 @ 10°C		[8]
	33.45 @ 20°C		[8]
	32.06 @ 30°C		[8]
	30.67 @ 40°C		[8]
	29.28 @ 50°C		[8]
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	0.001115 K^{-1}		[58]
Compressibility:	0.738 nPa^{-1} @ 25°C		[58]
Vapor diffusivity:	NA		
Solution diffusivity:	NA		
Electric dipole moment:	0		[8]
Ionization potential:	9.13 eV		[46]
Volume susceptibility:	-7.62×10^{-6} SI units @ 32°C		[85]
Speed of sound:	NA		
Heat of melting:	12.85 kJ/mol		[8]
Heat of vaporization:	35.585 kJ/mol		[58]
Heat of sublimation:	38.51 kJ/mol		[8]
Heat capacity @ 20°C:	0.155 kJ/(mol-K)	(liq)	[88]
@ 25°C	0.0941	(gas)	[8]
Heat of combustion:	-2432 kJ/mol @ 25°C	(liq)	[88]

Heat of formation:	-353.6	kJ/mol @ 25°C	(liq)	[8]
	-315.2		(gas)	[8]
Gibbs (free) energy:	-188.2	kJ/mol @ 25°C	(liq)	[8]
	-180.9		(gas)	[8]

Analytical chemistry: pKa = -2.92 in aqueous H_2SO_4 [58]
-1.83 @ 25°C in Water [58]

Electrochemical data: NA

Clay-organic interaction data: Basal spacings and delta values for complexes formed between Ca-montmorillonite and 1,4-dioxane together with calculated thickness and probable orientation of the intercalated molecules. Interlayer complexes of halloysite with 1,4-dioxane. Complexes formed with rehydrated halloysite obtained by washing the potassium acetate complex with water. [75]

Solubility: Miscible with water, alcohols, ether, acetone, benzene and most organic solvents.

Form: Colorless liquid; faint, pleasant, somewhat alcoholic odor; hygroscopic.

Use: In spray application, dipping, roller coating, tumbling, knifing, and brushing of natural and synthetic resin-based varnishes, lacquers, and paints; as a solvent for cellulose acetate, ethyl cellulose, benzyl cellulose, resins, fats, oils, waxes, greases, spirit-sol dyes, natural and synthetic resins, and many other organic as well as some inorganic compounds; as a wetting agent in textile processing, dye baths, and stain and printing compositions; as a degreaser; as a hydrating agent in preparation of histological slides; in manufacture of detergents and cleaning preparations; manufacture of polishing compounds; as a stabilizer for chlorinated solvents; in preparation of cosmetics and deodorants; in purification of drugs; as a working fluid for scintillation counter samples; as a solvent in pulping of wood.

Fire and Explosion Hazard: High.
Flash point: 12.2°C (CC) [63]
lel: 2.0%; uel: 22.2% [63]
Autoign. temp.: 180°C [63]
Highly flammable liquid with relatively broad explosion limits in air. Dangerous fire hazard when exposed to heat or flame. Flashback may occur along vapor trail. Potential explosion hazard when exposed to flame or by chemical reaction with oxidizers. Will produce peroxides in the presence of moisture. Dioxane containing peroxides should not be distilled to dryness because of the potential explosion of nonvolatile peroxides. Toxic gases and vapors (such as carbon monoxide) may be released in a fire. Contact with strong

oxidizing agents may cause fires and explosions. Fight fire with dry chemical, alcohol foam or CO_2. Water may be ineffective on fire.

Incompatible: With air. Violent reaction with (H_2+Raney Ni), $AgClO_4$. Avoid strong oxidizing agents.

Handling: Keep away from heat, sparks and flame. Avoid breathing vapor. Use in well-ventilated area with respirator. Prevent skin contact (PVA synthetic latex, neoprene, rubber, nitrile or polyethylene gloves, laboratory coat, face shield). Keep container tightly closed. Store secure poison area.

Health Effects: Dioxane can effect the body if it is inhaled, swallowed, or comes in contact with the eyes or skin. The vapor is an irritant to the eyes, nose, and throat. It may also cause drowsiness, loss of appetite, headache, nausea, vomiting, and stomach pain. Repeated exposure has resulted in death, the organs principally effected being the kidney and liver. The brain and lungs may also show acute edema. Prolonged skin exposure to the liquid may cause drying and cracking. Dioxane has been shown to induce tumors in animals. It is a weak animal carcinogen and suspected as a possible human carcinogen.

Toxicity: Moderate.
TWA: 25 ppm (skin)
CL: 1 ppm over a 30-min period (recommended)
IDLH: 200 ppm
Odor threshold: 1-170 ppm
Exposure: Mild transient irritation of the eyes, nose and throat has been reported for exposures of 300 ppm for 15 minutes. Exposure of animals to 0.1 to 3% (1000 to 30,000 ppm) dioxane vapor causes irritation of the eyes and nose, followed by narcosis and/or pulmonary edema and death. A worker exposed to 500 ppm via skin and inhalation routes for a week died. Damage was to the kidney, liver and brain.
Inhalation:
Non-lethal: 470 ppm/3 days
5500 ppm/1 min--Eye effects

ETHANOL C_2H_6O CAS RN: 64175

Syn: Absolute ethanol; alcohol; anhydrous alcohol; denatured alcohol; dehydrated alcohol; anhydrol; cologne spirit; cologne spirits; ethanol 200 proof; ethyl alcohol; ethyl alcohol anhydrous; ethyl hydrate; ethyl hydroxide; fermentation alcohol; grain alcohol; methylcarbinol; molasses alcohol; NCI-c03134; potato alcohol; spirits of wine.

Chemical formula: CH_3-CH_2OH Aliphatic Alcohol

Physical properties:

Relative molecular mass:	46.06904	
Specific gravity:	0.7893	[85]
Boiling point:	78.293°C	[58]
Melting point:	-114.49°C	[58]
Refractive index:	1.36143	[58]
Vapor pressure:	5.33 kPa @ 19°C	[63]
Vapor density:	1.59	[63]
Evaporation rate:	1.60	[58]
Relative permittivity:	41.8 @ -60°C	[85]
	25.07 @ 20°C	[20]
	24.55 @ 25°C	[8]
	22.14 @ 40°C	[20]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.179 W/(m-K) @ -20°C	[20]
	0.174 @ 0°C	[20]
	0.1673 @ 20°C	[85]
	0.132 @ 40°C	[20]
	0.156 @ 60°C	[20]
Electrical resistivity:	7.41 MOhm-m @ 25°C	[8]
Critical temperature:	240.77°C	[58]
Critical pressure:	6.148 MPa	[58]
Dynamic viscosity:	1.773 mPa-s @ 0°C	[85]
	1.466 @ 10°C	[85]
	1.200 @ 20°C	[85]
	1.003 @ 30°C	[85]
	0.834 @ 40°C	[85]
	0.702 @ 50°C	[85]
	0.592 @ 60°C	[85]
	0.504 @ 70°C	[85]
Kinematic viscosity:	2.246 $\mu m^2/s$ @ 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	[85]
	23.61 @ 10°C vapor	[85]
	22.75 @ 20°C vapor	[85]
	21.89 @ 30°C vapor	[85]

Contact angle:	NA on quartz			
	NA on calcite			
	NA on silica			
Thermal expansion coef.:	0.001096 K^{-1}			[58]
Compressibility:	0.963 nPa^{-1} @ 0°C			[85]
	1.030 @ 10°C			[85]
	1.098 @ 20°C			[85]
	1.180 @ 30°C			[85]
	1.261 @ 40°C			[85]
	1.360 @ 50°C			[85]
Vapor diffusivity:	10.2 $\mu m^2/s$ @ 0°C			[52]
Solution diffusivity:	1.28 nm^2/s in Water			[52]
Electric dipole moment:	5.64 x 10^{-30} C-m			[85]
Ionization potential:	10.49 eV (PI)			[85]
Volume susceptibility:	-7.23 x 10^{-6} SI units @ 20°C			[85]
Speed of sound:	1232.1 m/s @ 0°C			[20]
	1196.7 @ 10°C			[20]
	1161.8 @ 20°C			[20]
	1207 @ 25°C			[85]
	1127.6 @ 30°C			[20]
	1094.1 @ 40°C			[20]
	1061.2 @ 50°C			[20]
Heat of melting:	4.187 kJ/mol			[8]
Heat of vaporization:	38.75 kJ/mol			[8]
Heat of sublimation:	42.33 kJ/mol			[8]
Heat capacity @ 25°C:	0.1120 kJ/(mol-K)		(liq)	[8]
	0.0655		(gas)	[8]
Heat of combustion:	-1366.8 kJ/mol @ 25°C		(liq)	[58]
	-1409.4		(gas)	[58]
Heat of formation:	-277.2 kJ/mol @ 25°C		(liq)	[8]
	-234.6		(gas)	[8]
Heat of solution:	-10 kJ/mol @ 25°C			[86]
Gibbs (free) energy:	-174.3 kJ/mol @ 25°C		(liq)	[8]
	-168.0		(gas)	[8]

Analytical chemistry: pKa = 15.9 @ 25°C [58]
pKs = 19.1 [58]
pKh = -1.94 @ 25°C in aqueous H_2SO_4 [58]

Electrochemical data: NA

Clay-organic interaction data: Displacement of water by ethanol in the primary hydration shell around Ca^{2+}, Cu^{2+} 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^+, K^+, Ca^{2+} and increasing proportions of Li+ after heat treatment to 493 K for 24 hours and solvation with ethanol. 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.[75]

Solubility: Soluble in benzene; miscible with water, ether, acetone, chloroform, and with many organic liquids.

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.

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 is gasoline.

Fire and Explosion Hazard: High.
Flash point: 13.11°C (CC) [63]
lel: 3.3% @ 60°C; uel: 19.0% @ 60°C [63]
Autoign. temp.: 422.78°C [63]
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 foam, CO_2 or dry chemical. Can use water spray to "knock down" vapor.

Incompatible: Acetyl chloride, (Ag_2O+NH_4OH), BrF_5, $Ca(OCl)_2$, ClO_3, CrO_3, $Cr(OCl)_2$, (cyanuric acid+H_2O), H_2O_2, HNO_3, $(H_2O_2+H_2SO_4)$, $(I+CH_3OH+HgO)$, disulfuryl difluoride, oxidants, platinum, potassium, potassium-tert-butoxide, silver nitrate, silver oxide, [$Mn(ClO_4)_2$+2,2-dimethoxy propane], $Hg(NO_3)_2$, $HClO_4$, perchlorates, $(H_2S_2SO_4$+permanganates), $HMnO_4$, KO_2, $KOC(CH_3)_3$, $(Ag+HNO_3)$, $AgNO_3$, $AgClO_4$, NaH_3N_2, $UO_2(ClO_4)_2$.

Handling: Keep away from heat, sparks and flame. Keep container tightly closed, cool and away from flame. Avoid skin contact (neoprene, rubber, nitrile, butyl synthetic latex, polyethylene vinyl plastic or PVC coated nylon gloves, lab coat, goggles or face shield). Use in well-ventilated area. Respirator recommended. Keep containers tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet.

Health Effects: Ethyl alcohol 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.

Toxicity: Low.

TWA: 1000 ppm

Threshold odor: 10-5100 ppm

Exposure: Concentrations below 1000 ppm usually produce no signs of intoxication. Exposure to concentrations of 5000 to 10,000 ppm may result in irritation of the eyes and mucous membranes. If continued for an hour, stupor and drowsiness may result.

Oral:

Non-lethal: 50 mg/kg--Gastrointestinal tract effects
1430 μg/kg--CNS effects
256 gm/kg/12 weeks--effects on endocrine glandular system

ETHYLBENZENE C_8H_{10} CAS RN: 100414

Syn: Phenylethane; Ethylbenzol; NCI-c56393; EB.

Chemical formula: $C_6H_5CH_2CH_3$ Monocyclic Aromatic Hydrocarbon

Physical properties:

Relative molecular mass:	106.1670		
Specific gravity:	0.8670		[85]
Boiling point:	136.193°C		[58]
Melting point:	-94.975°C		[58]
Refractive index:	1.4959		[85]
Vapor pressure:	0.947 kPa @ 20°C		[37]
Vapor density:	3.66		[37]
Evaporation rate:	0.89		[58]
Relative permittivity:	2.412 @ 20°C		[8]
	2.238 @ 25°C		[10]
Loss tangent:	NA		
Relaxation time:	NA		
Thermal conductivity:	0.132 W/(m-K) @ 20°C		[85]
Electrical resistivity:	NA		
Critical temperature:	343.94°C		[8]
Critical pressure:	3.609 MPa		[8]
Dynamic viscosity:	0.6783 mPa-s @ 20°C		[58]
	0.6373 @ 25°C		[58]
Kinematic viscosity:	0.7824 $\mu m^2/s$ @ 20°C		
	0.7351 @ 25°C		
Surface tension:	29.20 mN/m @ 20°C vapor		[85]
	28.48 @ 25°C		[58]
	27.93 @ 30°C		[10]
	26.79 @ 40°C		[10]
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	NA		
Compressibility:	0.865 nPa^{-1}		[58]
Vapor diffusivity:	6.58 $\mu m^2/s$ @ 0°C		[52]
Solution diffusivity:	NA		
Electric dipole moment:	1.968 x 10^{-30} C-m		[8]
Ionization potential:	8.76 eV (PI)		[85]
Volume susceptibility:	-7.968 x 10^{-6} SI units @20°C		[85]
Speed of sound:	1351 m/s @ 20°C		[81]
Heat of melting:	9.190 kJ/mol		[8]
Heat of vaporization:	35.588 kJ/mol		[8]
Heat of sublimation:	42.29 kJ/mol		[8]
Heat capacity @ 25°C	0.1862 kJ/(mol-K)	(liq)	[85]
	0.1284	(gas)	[85]
Heat of combustion:	-4568 kJ/mol @ 20°C	(liq)	[85]
Heat of formation:	-12.48 kJ/mol @ 25°C	(liq)	[8]
	29.81	(gas)	[8]
Gibbs (free) energy:	130.67 kJ/mol @ 25°C	(liq)	[8]
	80.01	(gas)	[8]

Analytical chemistry: NA

Electrochemical data: [49], [62].

Clay-organic interaction data: NA

Solubility: Practically insoluble in water; soluble in ethanol; very soluble in ether; miscible with chloroform, benzene. (0.015g/100g water [37]).

Form: Colorless liquid; pungent, aromatic odor.

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; as a dielectric; naphtha constituent; anti-knock agent especially in airplane fuels; 4.6 wgt% in gasoline (high octane number). 18th highest volume chemical produced in U.S. (1979).

Fire and Explosion Hazard: High.
Flash point: 15°C (CC) [37]
lel: 1.0%; uel: 6.7% [37]
Autoign. temp.: 432°C [63]
Dangerous. Highly flammable liquid. Keep away from heat and open flame. Can react vigorously with oxidizing materials. Fire emits toxic gases and vapors, such as carbon monoxide. Fight fire with foam (most effective), CO_2 or dry chemical. Can use water spray to "knock down" vapor.

Incompatible: With strong oxidizing materials.

Handling: Keep away from heat or flame. Avoid breathing vapor. Use in well-ventilated area with respirator. Prevent repeated or prolonged skin contact (gloves [butyl synthetic latex, polyethylene and polyurethane coated nylon are best but still provide only marginal protection] and over clothing, lab coat, goggles or face shield). Keep container tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet.

Health effects: Both liquid and vapor ethylbenzene are an irritant to the eyes, skin and mucous membranes. 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 irritants are sufficient to cause workers to leave an atmosphere containing 0.5% of the vapor. Narcotic in high concentrations. Possible liver, kidney and pancreatic damage.

Toxicity: Moderate.
TWA: 100 ppm
STEL: 125 ppm
IDLH: 2000 ppm
Odor threshold: 0.25-200 ppm
Exposure: A concentration of 0.1% of the vapor in air is an irritant to the eyes, and a concentration of 0.2% is extremely irritating at first, then causes dizziness, irritation of the nose and throat and a sense of constriction in the chest. No data are available regarding the effect of chronic exposure.
External: 200 ppm--Eye irritation

ETHYLENE DIBROMIDE $C_2H_4Br_2$ CAS RN: 106934

Syn: 1,2-Dibromoethane; Bromofume 40; ENT 15349; ethylene bromide; EDB; sym-dibromoethane; alpha,beta-dibromoethane; 1,2-ethylene dibromide; glycol dibromide; NCI-c00522.

Chemical formula: $BrCH_2CH_2Br$
Aliphatic Polybrominated Hydrocarbon

Physical properties:

Relative molecular mass:	187.86176	
Specific gravity:	2.1792	[85]
Boiling point:	131.36°C	[85]
Melting point:	9.79°C	[85]
Refractive index:	1.5387	[85]
Vapor pressure:	1.467 kPa @ 20°C	[37]
Vapor density:	6.48	[63]
Evaporation rate:	NA	
Relative permittivity:	4.78 @ 25°C	[8]
	4.75 @ 30°C	[58]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	NA	
Electrical resistivity:	>50 MOhm-m @ 19°C	[58]
Critical temperature:	309.8°C	[58]
Critical pressure:	7.15 MPa	[58]
Dynamic viscosity:	2.438 mPa-s @ 0°C	[85]
	1.880 @ 15°C	[58]
	1.721 @ 20°C	[85]
	1.490 @ 30°C	[58]
	1.286 @ 40°C	[85]
	0.903 @ 70°C	[85]
	0.750 @ 82.2°C	[85]
	0.648 @ 99°C	[85]
Kinematic viscosity:	1.119 $\mu m^2/s$ @ 0°C	
	0.863 @ 15°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	[58]
	37.61 @ 30°C	[58]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.000943 K^{-1}	[58]
Compressibility:	0.650 nPa^{-1} @ 27°C	[58]
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	3.969 x 10^{-30} C-m	[58]
Ionization potential:	9.45 eV	[46]
Volume susceptibility:	-11.5 x 10^{-6} SI units @ 20°C	[85]

Speed of sound:	NA			
Heat of melting:	10.945	kJ/mol		[58]
Heat of vaporization:	36.35	kJ/mol		[58]
Heat of sublimation:	58.890	kJ/mol		[58]
Heat capacity @ 25°C:	0.1348	kJ/(mol-K)	(liq)	[85]
	0.0762		(gas)	[85]
Heat of combustion:	-1240.6	kJ/mol @ 25°C	(liq)	[58]
Heat of formation:	-81.2	kJ/mol @ 25°C	(liq)	[58]
	-38.33		(gas)	[58]
Gibbs (free) energy:	-20.9	kJ/mol @ 25°C	(liq)	[8]
	NA		(gas)	

Analytical chemistry: Koc = 58 [60]

Electrochemical data: NA

Clay-organic interaction data: Sorption of ethylene dibromide on soil and clay. [60]

Solubility: Slightly soluble in water; soluble in acetone, benzene; miscible with ethanol, ether. Emulsifiable. (0.429% in water @ 30°C [58]; 0.4g/100g water [63]).

Form: Colorless liquid or solid; mild, sweet chloroform-like odor.

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.

Fire and Explosion Hazard: Very low.
Flash point: not combustible
lel: not combustible
Autoign. temp.: not combustible
Nonflammable. 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.

Incompatible: Chemically active metals such as sodium, potassium, calcium, powdered aluminum, zinc, magnesium; liquid ammonia; strong oxidizers.

Handling: Keep away from light and heat. Use with adequate ventilation (fume hood). Avoid breathing vapors (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). Keep container tightly closed. Store in cool, dry, well-ventilated storage area away from heat.

Health effects: EDB is moderately toxic if inhaled, swallowed, or comes into contact with the eyes or skin. It may be absorbed through the skin. Contact with the skin may cause severe irritation and blistering. Inhalation may cause delayed pulmonary lesions. 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. EDB is a narcotic more poisonous than chloroform, a severe mucous membrane irritant and a hepatic toxin. It may be carcinogenic to humans.

Toxicity: Moderate.
TWA: 20 ppm
CL: 30 ppm
IDLH: 400 ppm Peak: 50 ppm for 5 min duration
Odor threshold: 10-25 ppm
Oral: Lethal dose: 90mg/kg

METHANOL CH_4O CAS RN: 67561

Syn: Carbinol; colonial spirit; columbian spirit; methylol; methyl alcohol; methyl hydroxide; monohydroxymethane; pyroxylic spirit; wood alcohol; wood naphtha; wood spirit.

Chemical formula: CH_3OH Aliphatic Alcohol

Physical properties:

Relative molecular mass:	32.04216	
Specific gravity:	0.7914	[85]
Boiling point:	64.546°C	[58]
Melting point:	-97.68°C	[58]
Refractive index:	1.3288	[85]
Vapor pressure:	12.93 kPa @ 20°C	[46]
Vapor density:	1.11	[88]
Evaporation rate:	2.10	[58]
	4.6	[5]
Relative permittivity:	37.98 @ 0°C	[8]
	33.64 @ 20°C	[8]
	32.70 @ 25°C	[8]
	29.73 @ 40°C	[20]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.216 W/(m-K) @ -20°C	[20]
	0.210 @ 0°C	[20]
	0.2023 @ 20°C	[85]
	0.198 @ 40°C	[20]
	0.193 @ 60°C	[20]
Electrical resistivity:	0.023 MOhm-m @ 18°C	[8]
Critical temperature:	240°C	[88]
Critical pressure:	7.954 MPa	[88]
Dynamic viscosity:	1.22 mPa-s @ -22.29°C	[85]
	0.820 @ 0°C	[85]
	0.623 @ 15°C	[85]
	0.597 @ 20°C	[85]
	0.547 @ 25°C	[85]
	0.510 @ 30°C	[85]
	0.456 @ 40°C	[85]
	0.403 @ 50°C	[85]
Kinematic viscosity:	1.54 $\mu m^2/s$ @ -22.9°C	
	1.04 @ 0°C	
	0.787 @ 15°C	
	0.754 @ 20°C	
	0.691 @ 25°C	
	0.644 @ 30°C	
	0.576 @ 40°C	
	0.509 @ 50°C	
Surface tension:	24.49 mN/m @ 0°C air	[85]
	22.61 @ 20°C air	[85]
	22.30 @ 25°C	[58]
	21.69 @ 30°C	[58]
	20.14 @ 50°C vapor	[85]

Contact angle:	NA on quartz			
	NA on calcite			
	NA on silica			
Thermal expansion coef.:	0.001196 K^{-1}			[58]
Compressibility:	1.078 nPa^{-1}	@ 0°C		[85]
	1.145	@ 10°C		[85]
	1.218	@ 20°C		[85]
	1.298	@ 30°C		[85]
	1.382	@ 40°C		[85]
	1.476	@ 50°C		[85]
Vapor diffusivity:	13.2 $\mu m^2/s$ @ 0°C			[52]
Solution diffusivity:	1.6 nm^2/s in water			[52]
Electric dipole moment:	5.67 x 10^{-30} C-m			[85]
Ionization potential:	10.84 eV (PI,PE)			[85]
Volume susceptibility:	-6.66 x 10^{-6} SI units @ 20°C			[85]
Speed of sound:	1189.2 m/s	@ 0°C		[20]
	1154.9	@ 10°C		[20]
	1121.2	@ 20°C		[20]
	1103	@ 25°C		[85]
	1088.2	@ 30°C		[20]
	1055.9	@ 40°C		[20]
	1024.0	@ 50°C		[20]
Heat of melting:	3.22 kJ/mol			[8]
Heat of vaporization:	34.5 kJ/mol			[8]
Heat of sublimation:	37.4 kJ/mol			[8]
Heat capacity @ 25°C:	0.08122 kJ/(mol-K)		(liq)	[8]
	0.04392		(gas)	[8]
Heat of combustion:	-726.51 kJ/mol	@ 25°C	(liq)	[58]
	-764.50		(gas)	[58]
Heat of formation:	-239.2 kJ/mol	@ 25°C	(liq)	[8]
	-201.2		(gas)	[8]
Heat of solution:	-0.64 kJ/mol	@ 25°C		[86]
Gibbs (free) energy:	-166.9 kJ/mol	@ 25°C	(liq)	[8]
	-162.5		(gas)	[8]

Analytical chemistry: Potential span = 800 mV [8]
pKs = 16.7 [8]

Electrochemical data: [3].

Clay-organic interaction data: 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. [75]

Solubility: Miscible with water, ethanol, ether, acetone, ketones, benzene, and most other organic solvents.

Form: Clear, colorless, very mobile liquid; slight alcohol odor when pure; repulsive, pungent odor from crude material.

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.

Fire and Explosion Hazard: High.
Flash point: 12°C (CC) [88]; 15°C (OC) [58]
lel: 6.0%; uel: 36.5% [88]
Autoign. temp.: 470°C [88]
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 react vigorously with oxidizing materials. Burns with nonluminous bluish flame. Fight fire with alcohol foam, dry chemical or CO_2. Water may be ineffective.

Incompatible: With beryllium dihydride, chloroform, cyanuric chloride, metals (especially magnesium), oxidants, potassium-tert-butoxide, bromine, sodium hypochlorite. Violent reaction with CrO_3, (I+ethanol+HgO), $Pb(ClO_4)_2$, $HClO_4$, P_2O_3, ($KOH+CHCl_3$), ($NaOH+CHCl_3$), nitric acid, hydrogen peroxide, alkylaluminum solutions, diethylzinc, 2,4,6-trichloror-s-triazine.

Handling: Keep away from heat, sparks and flame. Avoid skin contact (neoprene, rubber, nitrile, butyl synthetic latex, polyethylene, vinyl plastic, PVC coated nylon gloves, lab coat, safety goggles or face shield). Avoid breathing vapor. Use in well-ventilated area with supplied-air respirator. Do not use organic canister mask. Keep container tightly closed. Bond and ground container when transferring liquid. Store in cool, dry, well-ventilated flammable liquid storage area.

Health Effects: Methanol is a poison to the human system that possesses distinct narcotic properties. It is also a slight irritant to the mucous membranes. 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, 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. Methanol is a common air contaminant. It is used as a food additive permitted in foods for human consumption.

Toxicity: Moderate.
TWA: 200 ppm (skin)
STEL: 250 ppm
CL: 600 ppm
IDLH: 25000 ppm
Peak: 1000 ppm for 30 min duration
Odor threshold: 53-5900 ppm
Exposure: Death from ingestion of less than 30 mL has been reported. Usual fatal dose is 100 to 250 mL.
Oral:
Non-lethal: 340 mg/kg
Lethal dose: 100-250 mL
Inhalation: Non-lethal: 86000 mg/m^3

METHYLENE CHLORIDE CH_2Cl_2 CAS RN: 75092

Syn: Methane dichloride; dichloromethane; methylene bichloride; methylene dichloride; Freon 30; NCI-c50102.

Chemical formula: CH_2Cl_2 Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	84.9328			
Specific gravity:	1.3266			[85]
Boiling point:	39.64°C			[58]
Melting point:	-94.92°C			[58]
Refractive index:	1.4242			[85]
Vapor pressure:	46.66 kPa @ 20°C			[80]
Vapor density:	2.93			[63]
Evaporation rate:	27.5			[37]
	14.5			[5]
Relative permittivity:	9.08 @ 20°C			[85]
	8.93 @ 25°C			[58]
	8.649 @ 30°C			[58]
Loss tangent:	NA			
Relaxation time:	NA			
Thermal conductivity:	0.122 W/(m-K) @ 0°C			[85]
Electrical resistivity:	NA			
Critical temperature:	237.34°C			[10]
Critical pressure:	6.076 MPa			[10]
Dynamic viscosity:	0.449 mPa-s @ 15°C			[85]
	0.430 @ 20°C			[24]
	0.393 @ 30°C			[85]
Kinematic viscosity:	0.338 $\mu m^2/s$ @ 15°C			
	0.324 @ 20°C			
	0.296 @ 30°C			
Surface tension:	27.89 mN/m @ 20°C			[58]
	26.54 @ 30°C			[58]
Contact angle:	NA on quartz			
	NA on calcite			
	NA on silica			
Thermal expansion coef.:	0.001391 K^{-1}			[58]
Compressibility:	0.974 pPa^{-1} @ 25°C			[85]
Vapor diffusivity:	NA			
Solution diffusivity:	NA			
Electric dipole moment:	5.337 x 10^{-30} C-m			[8]
Ionization potential:	11.35 eV (PI)			[85]
Volume susceptibility:	-9.21 x 10^{-6} SI units @ 20°C			[85]
Speed of sound:	NA			
Heat of melting:	6.160 kJ/mol			[58]
Heat of vaporization:	27.98 kJ/mol			[58]
Heat of sublimation:	29.06 kJ/mol			[8]
Heat capacity @ 25°C:	0.1001 kJ/(mol-K)		(liq)	[30]
	0.0512		(gas)	[30]
Heat of combustion:	-557.89 kJ/mol @ 25°C		(liq)	[58]
	-447.2 @ 20°C		(gas)	[85]
Heat of formation:	-124.3 kJ/mol @ 25°C		(liq)	[8]
	-95.46		(gas)	[8]

Gibbs (free) energy:	-70.46	kJ/mol @ 25°C	(liq)	[8]
	-68.92		(gas)	[8]

Analytical chemistry: NA

Electrochemical data: [83].

Clay-organic interaction data: NA

Solubility: Slightly soluble in water; miscible with ethanol, ether. (1.32g/100g water @ 20°C [88]).

Form: Colorless liquid; pleasant, penetrating ether-like or chloroform- like odor.

Use: Solvent for cellulose acetate; degreasing and cleaning fluids; as solvent in food processing; plastics; paint removers; propellants; blowing agent for 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.

Fire and Explosion Hazard: Very low.
Flash point: none with normal testing methods [37]
lel: 12%; uel: 19% (at elevated temperatures) [37]
Autoign. temp.: 556°C [37]
Volatile. Vapor is not flammable and when mixed with air is not explosive. Reacts violently with Li, NaK, potassium-tert-butoxide. No explosion hazard under ordinary conditions. Dangerous when heated to decomposition as it emits highly toxic fumes of phosgene, hydrogen chloride, and carbon monoxide.

Incompatible: Contact with strong oxidizers, strong caustics, and 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.

Handling: Avoid heat and sunlight. Use in well-ventilated area (fume hood). Respirator for organic vapors and fumes should be worn to avoid excessive inhalation. Avoid skin contact (PVA synthetic latex or neoprene gloves, goggles and face shield, lab coat and apron). Keep container tightly closed. Store in secure poison area. Keep container out of sun and away from heat.

Health effects: Methylene chloride is very dangerous to the eyes. 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. Reported as causing cancer in laboratory animals.

Toxicity: Low.
TWA: 100 ppm
CL: 1000 ppm
IDLH: 5000 ppm
Peak: 2000 ppm for 5 min duration in 2 hr period
(NIOSH recommends TWA=75 ppm and CL=500 ppm)
Odor threshold: 25-320 ppm
Exposure: Up to 25,000 ppm concentration for 2 hr not lethal.
Concentrations of 7,200 ppm after 8 min causes parastesia of the extremities, after 16 min causes acceleration of the pulse to 100, during first 20 min causes congestion in the head, a sense of heat and slight irritation of the eyes. At a level of 2,300 ppm, there is no feeling of dizziness during 1 hr exposure, but nausea may occur after 30 min of exposure.
Inhalation:
Non-lethal: 500 ppm/1 yr at intervals--CNS effects
500 ppm/8 hr-- Effects on all blood elements

NAPHTHALENE $C_{10}H_8$ CAS RN: 91203

Syn: Naphthalin; naphthene; camphor tar; moth balls; moth flakes; naphthaline; NCI-c52904; white tar.

Chemical formula: $C_{10}H_8$ Polycyclic Aromatic Hydrocarbon

Physical properties:

Relative molecular mass:	128.1732		
Specific gravity:	1.162		[88]
Boiling point:	217.942°C (sublimes)		[58]
Melting point:	80.29°C		[58]
Refractive index:	1.5898 @ 85°C		[58]
	1.58212 @ 100°C		[88]
Vapor pressure:	0.0067 kPa @ 20°C (solid)		[37]
	0.997 @ 80.29°C (liq)		[58]
Vapor density:	4.42		[63]
Evaporation rate:	<<1		[37]
Relative permittivity:	2.54 @ 85°C		[85]
	2.52 @ 17-22°C (400 MHz)		[85]
Loss tangent:	NA		
Relaxation time:	NA		
Thermal conductivity:	0.377 W/(m-K) @ 0°C		[8]
Electrical resistivity:	25 MOhm-m @ 82°C		[8]
Critical temperature:	475.2°C		[8]
Critical pressure:	4.051 MPa		[8]
Dynamic viscosity:	0.967 mPa-s @ 80°C		[85]
	0.776 @ 100°C		[85]
Kinematic viscosity:	0.832 $\mu m^2/s$ @ 80°C		
	0.668 @ 100°C		
Surface tension:	31.8 mN/m @ 100°C		[58]
	28.8 @ 127°C air, vapor		[85]
	18.69 @ 218°C		[58]
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	NA		
Compressibility:	NA		
Vapor diffusivity:	5.13 $\mu m^2/s$ @ 0°C		[52]
Solution diffusivity:	NA		
Electric dipole moment:	0		[8]
Ionization potential:	8.12 eV (PI)		[85]
Volume susceptibility:	-10.3×10^{-6} SI units @ 20°C		[85]
Speed of sound:	NA		
Heat of melting:	18.991 kJ/mol		[8]
Heat of vaporization:	43.292 kJ/mol		[8]
Heat of sublimation:	73.69 kJ/mol		[8]
Heat capacity @ 25°C:	0.1658 kJ/(mol-K)	(sol)	[30]
	0.1343	(gas)	[30]
Heat of combustion:	-5156.95 kJ/mol @ 25°C	(sol)	[58]
	-5227.5	(gas)	[58]
Heat of formation:	75.362 kJ/mol @ 25°C	(sol)	[8]
	149.05	(gas)	[8]

Gibbs (free) energy:	201.18	kJ/mol @ 25°C	(sol)	[8]
	223.74		(gas)	[8]

Analytical chemistry: pKh = 4.0 @ 0°C in HF [58]

Electrochemical data: [19], [30], [31], [32], [34], [35], [48], [49], [51], [57], [59], [66] [72], [87].

Clay-organic interaction data: Intercalation with boiling air-dry samples of montmorillonite (saturated with Ca^{2+} or NH_4^+ ions). [75]

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. (0.003g/100g water @ 22°C [8]; 9.5/100 parts alcohol @ 19.5°C [8]; 46/100 parts benzene @ 16°C [8]; 69.16g/100g acetone @ 25°C [10]; 26.82g/100g Carbon tetrachloride @ 25°C [10]; 65.71g/100g benzene @ 25°C [10]; 57.12g/100g ether @ 25°C [10]; 19.82g/100g n-heptane @ 25°C [10]; 12.1g/100g ethanol @ 25°C [10]).

Form: White, crystalline flakes, powder, balls or cakes; aromatic coal- tar odor. Sublimes at room temperature.

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.

Fire and Explosion Hazard: Moderate.
Flash point: 78.9°C (CC); 87.8°C (OC) [86]
lel: 0.9%; uel: 5.9% [37]
Autoign. temp.: 526°C [37]
Combustible solid. Moderate fire hazard when exposed to heat or flame. Reacts with oxidizing materials. Reacts violently with CrO_3. Moderate explosion hazard in the form of dust when exposed to heat or flame. Fire may release dense acrid smoke and carbon monoxide. Fight fire with ordinary foam, CO_2, dry chemical. Molten naphthalene foams and splatters in contact with water.

Incompatible: With strong oxidizers, dinitrogen pentaoxide, CrO_3.

Handling: Keep away from heat, sparks and flame. Use in well-ventilated area (fume hood). Respirator recommended. Avoid skin contact (polyethylene, neoprene, PVA synthetic latex, nitrile or PVC coated nylon gloves and lab coat and boots, chemical goggles or face shield). Keep containers tightly closed. Store in cool, dry, well-ventilated area away from heat, sparks and flame.

Health effects: Poisoning may occur after ingestion of large dose, inhalation, or skin absorption of naphthalene. Systemic reactions include nausea, headache, diaphoresis, hematuria, anemia, fever, liver damage, vomiting, convulsions, and coma. 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.

Toxicity: Moderate.
TWA: 10 ppm
STEL: 15 ppm
IDLH: 500 ppm
Odor threshold: 0.003-0.3 ppm
External: 15 ppm--Eye irritation
Internal:
Lethal dose: 74 mg/kg

PHENOL C_6H_6O CAS RN: 108952

Syn: Carbolic acid; benzenol; hydroxybenzene; phenic acid; phenylic acid; phenyl hydrate; phenyl hydroxide; phenolyic alcohol; monohydroxybenzene; oxybenzene; NCI-c50124; Baker's P and S liquid and ointment.

Chemical formula: C_6H_5OH Monocyclic Aromatic Hydrocarbon

Physical properties:

Relative molecular mass:	94.1128	
Specific gravity:	1.0576 (sol)	[85]
	1.058 @ 41°C (liq)	[86]
Boiling point:	181.839°C	[58]
Melting point:	40.90°C	[58]
Refractive index:	1.5408 @ 41°C	[85]
Vapor pressure:	0.0480 kPa @ 20°C	[37]
Vapor density:	3.24	[37]
Evaporation rate:	<0.01	[37]
Relative permittivity:	11.60 @ 40°C	[58]
	9.78 @ 60°C	[85]
	4.3 @ 10°C (400 MHz)	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.149 W/(m-K) @ 30°C	[58]
	0.141 @ 75°C	[58]
Electrical resistivity:	>0.5882 Mohm-m @ 25°C	[8]
Critical temperature:	421.1°C	[8]
Critical pressure:	6.130 MPa	[8]
Dynamic viscosity:	12.7 mPa-s @ 18.3°C	[85]
	4.076 @ 45°C	[58]
	3.49 @ 50°C	[85]
	2.61 @ 60°C	[85]
	2.03 @ 70°C	[85]
	1.26 @ 90°C	[85]
Kinematic viscosity:	12.01 $\mu m^2/s$ @ 18.3°C	
	3.854 @ 45°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	[85]
	39.88 @ 30°C air, vapor	[85]
	37.66 @ 50°C	[11]
	36.57 @ 60°C	[11]
	35.51 @ 70°C	[11]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	NA	
Compressibility:	0.561 nPa^{-1} @ 46°C	[85]
	0.605 @ 60°C	[85]
	0.678 @ 80°C	[85]
Vapor diffusivity:	NA	

Solution diffusivity:	0.2 nm^2/s	in i-Amyl alcohol		[52]
	1.68	in Benzene		[52]
	3.7	in Carbon disulfide		[52]
	2.0	in Chloroform		[52]
	0.89	in Ethanol		[52]
	3.9	in Ethyl ether		[52]
Electric dipole moment:	4.837 x 10^{-30} C-m			[8]
Ionization potential:	8.51 eV (PI)			[85]
Volume susceptibility:	-8.48 x 10^{-6} SI units @ 45°C			[85]
Speed of sound:	NA			
Heat of melting:	11.52 kJ/mol			[8]
Heat of vaporization:	40.73 kJ/mol			[8]
Heat of sublimation:	68.71 kJ/mol			[8]
Heat capacity @ 25°C:	0.1348 kJ/(mol-K)		(sol)	[8]
	0.1275		(liq)	[8]
	0.1036		(gas)	[8]
Heat of combustion:	-3056 kJ/mol	@ 25°C	(sol)	[85]
Heat of formation:	-165.1 kJ/mol	@ 25°C	(sol)	[8]
	-158.3		(liq)	[8]
	-96.42		(gas)	[8]
Gibbs (free) energy:	-50.45 kJ/mol	@ 25°C	(sol)	[8]
	-46.14		(liq)	[8]
	-32.91		(gas)	[8]

Analytical chemistry: pKa = 9.686 @ 20°C in Water [58]
= 9.99 @ 25°C in Water [8]
= 9.658 @ 30°C in Water [58]
= 14.0 in methanol [8]

Electrochemical data: [2], [13], [22], [56], [68], [74], [77], [78].

Clay-organic interaction data: Interlayer expansions in vermiculite due to intercalated phenols [75]. Water molecules reacting as bases and accepting protons from acids through hydrogen bounding by sorption of phenol on Al-montmorillonite [89].

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 [8]. (8.2g/100g water @ 15°C [8]).

Form: Colorless, acicular crystals or white, crystalline mass which turns pink or red if not perfectly pure; characteristic sweet, tarry, odor; burning taste; weak organic acid.

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.

Fire and Explosion Hazard: Moderate.
Flash point: 79.4°C (CC); 85°C (OC) [86]
lel: 1.7%; uel: 8.6% [37]
Autoign. temp.: 715°C [37]
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 foam, CO_2, dry chemical or water spray.

Incompatible: Contact with strong oxidizers (especially calcium hypochlorite); formaldehyde, $NaNO_2$, $NaNO_3$/trifluoroacetic acid. Reacts violently with ($AlCl_3$+nitrobenzene), butadiene, peroxydisulfuric acid, peroxymonosulfuric acid.

Handling: Keep away from heat, sparks and flame. Avoid breathing vapor. Use in well-ventilated area (fume hood). Use chemical cartridge respirator at concentrations up to 50 ppm. Above that use self-contained breathing apparatus. Fresh air mask recommended. Do not get in eyes, skin or clothing. Prevent skin contact (neoprene, rubber, latex or nitrile gloves, lab coat and apron, safety goggles and face shield). Keep container tightly closed. Store in cool, dry, well-ventilated, flammable liquid storage area or cabinet.

Health effects: 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.

Toxicity: High.
TWA: 5 ppm (skin) (vapors can be absorbed through skin)
STEL: 10 ppm
IDLH: 100 ppm
Odor threshold: 0.05-5 ppm
Oral:
Lethal dose: 140 mg/kg
1-10 g

QUINOLINE C_9H_7N CAS RN: 91225

Syn: 1-Azanaphthalene; 1-benzanine; benzo(b)pyridine; chinoline; leucol; leucoline; USAF EK-218.

Chemical formula: C_9H_7N Quinoline Alkaloid

Physical properties:

Relative molecular mass:	129.16128	
Specific gravity:	1.0929	[85]
Boiling point:	237.1°C	[58]
Melting point:	-14.85°C	[58]
Refractive index:	1.6273	[58]
Vapor pressure:	0.0112 kPa @ 25.16°C	[58]
Vapor density:	4.45	[63]
Evaporation rate:	NA	
Relative permittivity:	9.00 @ 25°C	[85]
	5.05 @ 238°C	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	NA	
Electrical resistivity:	0.45 MOhm-m @ 25°C	[8]
Critical temperature:	521.3°C	[58]
Critical pressure:	5.8 MPa	[58]
Dynamic viscosity:	4.354 mPa-s @ 15°C	[8]
	3.145 @ 25°C	[58]
	2.997 @ 30°C	[58]
Kinematic viscosity:	3.984 $\mu m^2/s$ @ 15°C	
	2.878 @ 25°C	
	2.742 @ 30°C	
Surface tension:	45.65 mN/m @ 20°C	[58]
	44.82 @ 30°C	[58]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	NA	
Compressibility:	NA	
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	7.64×10^{-30} C-m	[85]
Ionization potential:	NA	
Volume susceptibility:	-9.16×10^{-6} SI units @ 20°C	[85]
Speed of sound:	NA	
Heat of melting:	10.79 kJ/mol	[58]
Heat of vaporization:	49.71 kJ/mol	[58]
Heat of sublimation:	NA	
Heat capacity @ 25°C:	0.199 kJ/(mol-K) (liq)	[85]
Heat of combustion:	-4700.72 kJ/mol @ 25°C (liq)	[58]
Heat of formation:	156.3 kJ/mol @ 25°C (liq)	[8]
Gibbs (free) energy:	275.9 kJ/mol @ 25°C (liq)	[8]

Analytical chemistry: pK = 9.5 [88]
pKa = 4.80 (protonated cation) @ 20°C in Water [85]
pKh = 4.94 @ 25°C in aqueous ethanol [58]

Electrochemical data: [7], [17], [18], [87].

Clay-organic interaction data: NA

Solubility: Soluble in water; miscible with ethyl alcohol, ether, acetone, benzene, carbon disulfide. Dissolves sulfur, phosphorus, arsenic trioxide. (0.6/100 parts H_2O [8]).

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; weak base (neutral to phenolphthalein); forms water soluble salts with strong acids.

Use: Manufacture of dyes; preparation of hydroxyquinoline sulfate (niacin); as preservative for anatomical specimens; solvent for resins, terpenes.

Fire and Explosion Hazard: Low.
Flash point: 107.2°C (CC) [86]
lel: NA ; uel: NA
Autoign. temp.: 480°C [63]
Slight fire hazard when exposed to heat. Violent reaction with perchromates. Dangerous when heated to decomposition as it emits toxic fumes of nitrogen oxides. Fight fire with water, dry chemical, foam or CO_2.

Incompatible: Strong oxidizing agents; dinitrogen tetraoxide; linseed oil; thionyl chloride; maleic anhydride. May attack some forms of plastics.

Handling: Avoid moisture, light and heat. Do not get in eyes, on skin or on clothing (rubber gloves, lab coat and apron, goggles and shield). Do not breath vapor. Use in well-ventilated area (fume hood). Self-contained breathing apparatus or chemical cartridge respirator recommended. Keep container tightly closed. Keep product out of light. Store in secure poison area.

Health Effects: Quinoline vapors may irritate the skin, eyes and mucous membranes. Inhalation may cause headaches, dizziness and nausea. Contact with eyes and skin causes irritation. Potential to induce liver carcinoma.

Toxicity: Unknown.
TWA: 0.1 (skin) (American Industrial Hygiene Association)
Odor threshold: 0.16-71 ppm

TETRACHLOROETHENE C_2Cl_4 CAS RN: 127184

Syn: Tetrachloroethylene; 1,1,2,2-tetrachloroethylene; carbon dichloride; carbon bichloride; Dow-per; ethylene tetrachloride; Perclene; NCI-c04580; perchloroethylene (PCE); perchlorethylene; Nema; Tetracap; Tetropil; Didakene; Ankilostin; Perk.

Chemical formula: $Cl_2C=CCl_2$ Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	165.8340		
Specific gravity:	1.6227		[85]
Boiling point:	121.07°C		[58]
Melting point:	-22.35°C		[58]
Refractive index:	1.50576		[58]
Vapor pressure:	1.87 kPa @ 20°C		[37]
Vapor density:	5.83		[37]
Evaporation rate:	2.8		[37]
	2.10		[58]
Relative permittivity:	2.30 @ 25°C		[8]
Loss tangent:	NA		
Relaxation time:	NA		
Thermal conductivity:	0.162 W/(m-K) @ 20°C		[85]
Electrical resistivity:	NA		
Critical temperature:	347.1°C		[11]
Critical pressure:	4.491 MPa		[11]
Dynamic viscosity:	0.932 mPa-s @ 15°C		[58]
	0.798 @ 30°C		[58]
Kinematic viscosity:	0.574 $\mu m^2/s$ @ 15°C		
	0.492 @ 30°C		
Surface tension:	32.86 mN/m @ 15°C		[58]
	31.74 @ 20°C vapor		[85]
	31.30 @ 25°C		[58]
	30.81 @ 30°C		[11]
	30.20 @ 40°C		[11]
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	0.00102 K^{-1}		[58]
Compressibility:	0.756 nPa^{-1} @ 25°C		[85]
Vapor diffusivity:	NA		
Solution diffusivity:	NA		
Electric dipole moment:	0		[8]
Ionization potential:	9.32 eV (PI)		[85]
Volume susceptibility:	-10.1×10^{-6} SI units @ 15°C		[85]
Speed of sound:	NA		
Heat of melting:	10.47 kJ/mol		[8]
Heat of vaporization:	34.75 kJ/mol		[8]
Heat of sublimation:	39.4 kJ/mol		[8]
Heat capacity @ 25°C:	0.1465 kJ/(mol-K)	(liq)	[58]
	0.0950	(gas)	[8]
Heat of combustion:	-679.9 kJ/mol @ 25°C	(liq)	[58]
	-772.5	(gas)	[20]

Heat of formation:	-52.3	kJ/mol @ 25°C	(liq)	[58]
	-12.1		(gas)	[58]
Gibbs (free) energy:	NA		(liq)	
	20.52	kJ/mol @ 25°C	(gas)	[8]

Analytical chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Almost insoluble in water; miscible in ethanol, ether, benzene, chloroform and oils. (0.015g/100g water @ 20°C [37]).

Form: Colorless liquid; ether-like or chloroform-like odor; extremely stable; resists hydrolysis.

Use: Principle commercial dry cleaning solvent; degreasing metals; drying agent; chemical manufacturing of fluorocarbons; heat transfer medium; grain fumigant; solvents for fats, greases, waxes, rubber, gums, caffeine from coffee; remove soot from industrial boilers; manufacture of paint removers, printing inks, trichloroacetic acid.

Fire and Explosion Hazard: Very low.
Flash point: none [37]
lel: not combustible [37]
Autoign. temp.: not combustible.
Nonflammable. Dangerous if heated to decomposition as it emits highly toxic fumes of chlorides, phosgene, and carbon monoxide. PCE is extremely stable and resists hydrolysis. It may be handled in the presence or absence of air, water, and light with any of the common construction materials at temperatures up to 140°C.

Incompatible: Reacts with strong oxidizers and chemically active metals, such as barium, lithium and beryllium; N_2O_4; NaOH.

Handling: Avoid heat, sources of ignition and flame. Do not get in eyes, on skin or on clothing. Avoid breathing vapors. Use with adequate ventilation (fume hood). Avoid repeated or prolonged skin contact (plastic gloves, lab coat and apron, face shield or chemical goggles). Keep container tightly closed. Store in secure poison area.

Health effects: Not corrosive or dangerously acutely reactive, but toxic by inhalation, by prolonged or repeated contact with the skin or mucous membranes, or when ingested by mouth.

Contact with skin or eyes may cause severe irritation or burns. PCE can cause dermatitis, particularly after repeated or prolonged contact with the skin. Upon ingestion it causes irritation of the gastrointestinal tract, which, in turn, causes nausea, vomiting, diarrhea and bloody stools. Inhalation of vapors may cause coughing, chest pains, difficulty breathing or unconsciousness. The symptoms of acute intoxication from PCE are the results of its effects on the nervous system. Narcotic in high concentrations. Chronic effects of overexposure may include liver and/or kidney damage, and embryotoxicity. PCE is a common air contaminant.

Toxicity: Moderate.
TWA: 50 ppm
STEL: 200 ppm
CL: 200 ppm
IDLH: 500 ppm
Peak: 300 ppm for 5 min duration in a 3 hr period
Odor threshold: 5-50 ppm
Exposure: Exposures to higher than 200 ppm cause irritation, lachrymation and burning of the eyes and irritation of the nose and throat.
Inhalation:
Non-lethal: 96 ppm/7 hr--Liver and kidney damage
280 ppm/2 hr--Eye irritation
600 ppm/10 min--CNS effects

TOLUENE C_7H_8 CAS RN: 108883

Syn: Methylbenzene; phenylmethane; methylbenzol; Methacide; NCI-c07272; toluol.

Chemical formula: $CH_3C_6H_5$ Monocyclic Aromatic Hydrocarbon

Physical properties:

Relative molecular mass:	92.1402	
Specific gravity:	0.8669	[85]
Boiling point:	110.630°C	[58]
Melting point:	-94.991°C	[58]
Refractive index:	1.49693	[58]
Vapor pressure:	2.93 kPa @ 20°C	[37]
Vapor density:	3.14	[37]
Evaporation rate:	1.90	[5]
Relative permittivity:	2.438 @ 0°C	[85]
	2.379 @ 25°C	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.146 W/(m-K) @ -20°C	[20]
	0.141 @ 0°C	[20]
	0.136 @ 20°C	[20]
	0.131 @ 40°C	[20]
	0.126 @ 60°C	[20]
	0.118 @ 80°C	[85]
Electrical resistivity:	>1 x 10^6 MOhm-m	[8]
Critical temperature:	318.57°C	[8]
Critical pressure:	4.109 MPa	[8]
Dynamic viscosity:	0.772 mPa-s @ 0°C	[85]
	0.590 @ 20°C	[85]
	0.5525 @ 25°C	[58]
	0.526 @ 30°C	[85]
	0.4928 @ 35°C	[58]
	0.471 @ 40°C	[85]
	0.354 @ 70°C	[85]
Kinematic viscosity:	0.891 $\mu m^2/s$ @ 0°C	
	0.681 @ 20°C	
	0.6373 @ 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	[85]
	28.5 @ 20°C vapor	[85]
	27.92 @ 25°C	[58]
	27.33 @ 30°C	[58]
	26.15 @ 40°C	[10]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.001067 K^{-1}	[58]

Compressibility:	0.797 nPa^{-1} @ 0°C		[85]
	0.844 @ 10°C		[85]
	0.894 @ 20°C		[85]
	0.949 @ 30°C		[85]
	1.014 @ 40°C		[85]
Vapor diffusivity:	7.6 $\mu m^2/s$ @ 0°C		[52]
	8.8 @ 30°C		[52]
Solution diffusivity:	2.09 nm^2/s in n-Decane		[52]
	1.38 in n-Dodecane		[52]
	3.72 in n-Heptane		[52]
	4.21 in n-Hexane		[52]
	1.02 in n-Tetradecane		[52]
Electric dipole moment:	1.501×10^{-30} C-m		[8]
Ionization potential:	8.82 eV		[46]
Volume susceptibility:	-7.765×10^{-6} SI units @20°C		[85]
Speed of sound:	1227.2 m/s @ 20.5°C		[11]
Heat of melting:	6.640 kJ/mol		[8]
Heat of vaporization:	33.20 kJ/mol		[8]
Heat of sublimation:	38.02 kJ/mol		[8]
Heat capacity @ 25°C:	0.1561 kJ/(mol-K)	(liq)	[85]
	0.1038	(gas)	[85]
Heat of combustion:	-3949 kJ/mol @ 20°C	(liq)	[85]
Heat of formation:	12.02 kJ/mol @ 25°C	(liq)	[8]
	50.03	(gas)	[8]
Gibbs (free) energy:	113.8 kJ/mol @ 25°C	(liq)	[8]
	122.1	(gas)	[8]

Analytical chemistry: pKh = 6.3 @ 0°C in HF [58]

Electrochemical data: [35], [48], [49], [68].

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. [75]

Solubility: Almost insoluble in water; soluble in acetone; miscible in ethanol, chloroform, ether, benzene, glacial acetic acid, carbon disulfide. (0.05g/100g water @ 20°C [37]).

Form: Colorless liquid; pungent, aromatic, benzene-like odor. Commercial grades may contain up to 25% benzene.

Use: In manufacturing benzoic acid, benzaldehyde, explosives (TNT), dyes, and many other organic compounds; as a solvent for paints, lacquers, neoprene, gums, resins; in the extraction of various principles from plants; aviation and high octane blending stock; adhesive solvent in plastics; dilutor and thinner; detergents; scintillation counters; 16th highest-volume chemical produced in U.S. (1979).

Fire and Explosion Hazard: Moderate.
Flash point: 4.4°C (CC); 12.8°C (OC) [86]
lel: 1.27%; uel: 7.0% [86]
Autoign. temp.: 536°C [86]
Only slightly flammable when exposed to heat, flame or oxidizers despite low flash point. Moderately dangerous when heated as it emits irritating fumes (carbon monoxide and carbon dioxide). Can react vigorously with oxidizing materials. Fight small fires with CO_2 or dry chemical; ordinary foam for large fires. Water may be ineffective.

Incompatible: Contact with strong oxidizers; BrF_3, 1,3-dichloro-dimethyl-2,4-imidazolidin-2,4-dione, N_2O_4, nitric acid, sulfuric acid, tetranitromethane, UF_6. Will attack some forms of plastics, rubber, and coatings.

Handling: Keep away from heat sparks and flame. Avoid breathing vapor. Use with adequate ventilation (fume hood). Respirator recommended. Avoid repeated or prolonged skin contact (PVA synthetic latex gloves, lab coat, goggles or face shield). Keep container tightly closed. Store in cool, dry, well-ventilated flammable liquid storage area or cabinet. Store in secure poison area.

Health effects: Toluene is derived from coal tar, and commercial grades usually contain small quantities of benzene as an impurity. Inhalation of vapors may cause nausea, vomiting, headache or unconsciousness. Acute poisoning resulting from high concentrations of the vapors are rare. In the few cases of acute toluene poisoning reported, the effect has been that of a narcotic. Eye and skin irritation; upper respiratory tract irritation. Chronic effects of overexposure may include liver and/or kidney damage, and cardiovascular effects. Toluene is a common air contaminant.

Toxicity: Moderate.
TWA: 100 ppm
STEL: 150 ppm
CL: 200 ppm
IDLH: 2000 ppm
Peak: 500 ppm for 10 min duration
Odor threshold: 0.17-100 ppm (fatigue level at 300-400 ppm)
Exposure: Exposure to concentrations up to 200 ppm produce few symptoms. At 200-500 ppm, headache, nausea, eye irritation, loss of appetite, a bad taste, lassitude, impairment of coordination and reaction time are reported. With higher concentrations, the above complaints are increased and in addition, anemia, leucopenia and enlarged liver may be found in rare cases.
External: 300 ppm--Eye irritation
Inhalation:
Non-lethal: 200 ppm--CNS effects
100 ppm--Psychotropic effects

1,1,1-TRICHLOROETHANE $C_2H_3Cl_3$ CAS RN: 71556

Syn: Methyl chloroform; chloroethene; chlorothane nu; chlorothene; methyltrichloromethane; NCI-c04626; alpha-trichloroethane.

Chemical formula: CH_3CCl_3 Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	133.4047		
Specific gravity:	1.3390		[85]
Boiling point:	74.083°C		[58]
Melting point:	-30.4°C		[58]
Refractive index:	1.4379		[85]
Vapor pressure:	13.33 kPa @ 20°C		[37]
Vapor density:	4.45		[37]
Evaporation rate:	12.8		[37]
Relative permittivity:	7.953 @ 0°C		[8]
	7.68 @ 20°C		[8]
Loss tangent:	NA		
Relaxation constant:	NA		
Thermal conductivity:	NA		
Electrical resistivity:	1.37 MOhm-m		[58]
Critical temperature:	272°C		[58]
Critical pressure:	4.3		[58]
Dynamic viscosity:	0.903 mPa-s @ 15°C		[8]
	0.795 @ 25°C		[58]
	0.725 @ 30°C		[58]
Kinematic viscosity:	0.674 $\mu m^2/s$ @ 15°C		
	0.594 @ 20°C		
	0.541 @ 30°C		
Surface tension:	26.17 mN/m @ 15°C		[58]
	25.39 @ 20°C		[11]
	24.11 @ 30°C		[11]
	22.87 @ 40°C		[11]
Contact angle:	NA on quartz		
	NA on calcite		
	NA on silica		
Thermal expansion coef.:	NA		
Compressibility:	NA		
Vapor diffusivity:	NA		
Solution diffusivity:	NA		
Electric dipole moment:	5.971 x 10^{-30} C-m		[8]
Ionization potential:	NA		
Volume susceptibility:	NA		
Speed of sound:	NA		
Heat of melting:	2.350 kJ/mol		[58]
Heat of vaporization:	29.708 kJ/mol		[58]
Heat of sublimation:	32.5 kJ/mol		[8]
Heat capacity @ 25°C:	0.1439 kJ/(mol-K)	(liq)	[85]
	0.0937	(gas)	[85]
Heat of combustion:	-1108.05 kJ/mol @ 25°C	(liq)	[58]
Heat of formation:	-178.82 kJ/mol @ 25°C	(liq)	[58]
	-142.3	(gas)	[58]

Gibbs (free) energy:	NA		(liq)	
	-76.24	kJ/mol @ 25°C	(gas)	[8]

Analytical chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Almost insoluble in water; soluble in acetone, benzene, carbon tetrachloride, methanol; miscible in ethanol, ether; absorbs some water. (0.07g/100g water @ 20°C [37]; 0.132g/100g water @ 20°C [58]).

Form: Colorless liquid; mild odor like chloroform; ketones, alcohols, esters, or nitrogen compounds may be added as stabilizers or inhibitors.

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.

Fire and Explosion Hazard: Very low.
Flash point: none with normal testing methods [37]
lel: 7%; uel: 16% [37]
Autoign. temp.: 500°C [37]
Nonflammable but dangerous. Fire emits toxic fumes of hydrogen chloride, chlorine, phosgene, and carbon monoxide. Contact with strong caustics, strong oxidizers, and chemically active metals may cause fire or explosion. Fight fire with foam, dry chemical or CO_2.

Incompatible: Water, strong bases, aluminum and magnesium powders, chemically active metals strong oxidizing agents and strong bases. Reacts violently with N_2O_4, O_2, O_2 liquid, Na, NaOH, Na-K alloy.

Handling: Avoid moisture, insufficient inhibitor, heat, flame, other sources of ignition, sunlight and ultraviolet light. Avoid breathing vapor. Use with adequate ventilation (fume hood). Organic vapor-acid gas canister respirator should be worn. Avoid repeated or prolonged skin contact (neoprene or polyvinyl alcohol gloves, lab coat and boots, chemical safety goggles and face shield). Keep container tightly closed. Suitable for general chemical storage.

Health effects: Short-term exposure to vapor may cause headache, dizziness, drowsiness, unconsciousness, irregular heart beat and death. 1,1,1-Trichlroethane may cause irritation if splashed in the eyes. Prolonged or repeated skin contact may cause irritation, dermatitis. Chronic effects of overexposure may include liver and/or kidney damage. Narcotic in high concentrations. Causes a proarrhythmic activity which sensitizes the heart to epinephrine induced arrythmias. This sometimes may cause a cardiac arrest if massively inhaled.

Toxicity: Moderate.
TWA: 350 ppm
STEL: 450 ppm
CL: 350 ppm
IDLH: 1000 ppm
Peak: 800 ppm for 5 min in a 2 hr period
Odor threshold: 20-400 ppm
Exposure: A 5-minute exposure to 5000 ppm can be expected to produce marked incoordination and anesthesia. Prolonged exposure to this concentration may cause coma. Exposure to concentrations in excess of 1000 ppm for 15 minutes, or 2000 ppm for 5 minutes, can be expected to produce a disturbance of equilibrium in the majority of adults. Above 1700 ppm, minor disturbances of equilibrium have been observed, with complaints of headache and lassitude. In exposures to 500 ppm, no effects other than slight eye irritation were noted.
External:
Non-lethal: 450 ppm/8 hr--Eye irritation
Inhalation:
Non-lethal: 920 ppm/70 min--CNS effects
350 ppm--Psychotropic effects
Lethal dose: 27 gm/m^3/10 min
Oral:
Non-lethal 670 mg/kg--Gastrointestinal tract effects

TRICHLOROETHENE C_2HCl_3 CAS RN: 79016

Syn:Trichloroethylene; 1,1,2-trichloroethylene; TCE; ethinyl trichloride; Triclene; Trielene; Trichloran; Tricloren; Trimar; Triline; Tri; Trethylene; acetylene trichloride; Vextrol; NCI-co4546; Dow-tri; ethylene trichloride; Westrosol; Chlorylen; Gemalgene; Germalene; Benzinol; Circosolv; Flekflip; Blacosolv; 1,1-dichloro-2-chloroethylene; Algylene

Chemical formula: $ClCH=CCl_2$ Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	131.3889	
Specific gravity:	1.4642°C	[85]
Boiling point:	87.19°C	[58]
Melting point:	-86.4	[58]
Refractive index:	1.4773	[85]
Vapor pressure:	7.73 kPa @ 20°C	[5]
Vapor density:	4.53	[63]
Evaporation rate:	4.46	[58]
Relative permittivity:	3.42 @ 16°C	[8]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.116 W/(m-K) @ 20°C	[85]
Electrical resistivity:	1.25 MOhm-m @ 20°C	[58]
Critical temperature:	298°C	[5]
Critical pressure:	4.91 MPa	[5]
Dynamic viscosity:	0.566 mPa-s @ 20°C	[58]
	0.532 @ 25°C	[58]
	0.517 @ 30°C	[58]
Kinematic viscosity:	0.387 $\mu m^2/s$ @ 20°C	
	0.363 @ 25°C	
	0.353 @ 30°C	
Surface tension:	29.5 mN/m @ 20°C	[58]
	28.8 @ 25°C	[58]
	27.94 @ 30°C	[11]
	26.76 @ 40°C	[11]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.00117 K^{-1}	[58]
Compressibility:	0.857 nPa^{-1} @ 25°C	[85]
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	3.002 x 10^{-30} C-m	[8]
Ionization potential:	9.45 eV (PI)	[85]
Volume susceptibility:	-9.22 x 10^{-6} SI units @ 20°C	[85]
Speed of sound:	NA	
Heat of melting:	NA	
Heat of vaporization:	31.5 kJ/mol	[8]
Heat of sublimation:	34.3 kJ/mol	[8]
Heat capacity @ 25°C:	0.1218 kJ/(mol-K) (liq)	[30]
	0.0794 (gas)	[30]
Heat of combustion:	-962.37 kJ/mol @ 18°C (liq)	[58]

Heat of formation:	-42.3	kJ/mol @ 25°C	(liq)	[58]
	-5.862		(gas)	[8]
Gibbs (free) energy:	NA		(liq)	
	19.89	kJ/mol @ 25°C	(gas)	[8]

Analytical chemistry: Koc = 195 [60]

Electrochemical data: NA

Clay-organic interaction data: Sorption of trichloroethylene on soil and clay [60].

Solubility: Slightly soluble in water; soluble in acetone; miscible with ethanol, ether, chloroform. Dissolves most fixed and volatile oils. (0.1g/100g water @ 25°C [8].

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.

Fire and Explosion Hazard: Very low.
Flash point: not combustible.
lel: 8.0%; uel: 10.5% [86]
Autoign. temp.: 420°C [63]
Nonflammable 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 phosgene and hydrogen chloride. TCE or its vapors in contact with flames or hot glowing surfaces may form corrosive acids. Fight fire with dry chemical, CO_2, foam or water fog.

Incompatible: Can react violently with Al, Ba, Be, N_2O_4, Li, Mg, liquid O_2, O_3, KOH, KNO_3, Na, NaOH, Ti; chemically active metals and strong bases.

Handling: Keep away from heat, light, sources of ignition and flame. Avoid breathing vapor. Use with adequate ventilation (fume hood). Respirator recommended. Avoid skin contact (PVA synthetic latex gloves, lab coat, chemical safety goggles, face shield). Preserve in sealed, light-resistant ampoules or in non-breakable, light-resistant glass tubes. Keep container tightly closed. Store in secure poison area.

Health effects: Trichloroethene is a strong skin and eye irritant. Readily absorbed from the lungs and gastrointestinal tract but can also be absorbed through the skin. 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 effects of overexposure may result in lung/respiratory, liver and or kidney damage, blood cell disorders, cardiovascular effects (ventricular fibrillation). A common air contaminant. A food additive permitted in food for human consumption. Reported as causing cancer in laboratory animals

Toxicity: Moderate.
TWA: 50 ppm
STEL: 200 ppm
CL: 150 ppm
IDLH: 1000 ppm
Peak: 300ppm for 15 min in a 2 hr period
Odor threshold: 18-100 ppm
Exposure: Symptoms of illness begin to occur at 800 ppm; severe toxic effects at 2000 ppm; and full narcosis at 2500 to 6000 ppm.
External: 5 ppm--Eye irritation
Inhalation:
Non-lethal: 160 ppm/83 min--CNS effects
110 ppm/8 hr--Skin, eye, mucous membrane irritation
Lethal dose: 2900 ppm
Oral:
Non-lethal: 812 mg/kg--Liver and kidney damage
Lethal dose: 7 g/kg

VINYL CHLORIDE C_2H_3Cl CAS RN: 75014

Syn: Chloroethylene; chloroethene; ethylene monochloride; monochloroethene; monochloroethylene; vinyl chloride monomer; vinyl c monomer, 1-chloroethylene; MVC

Chemical formula: CH_2=CHCl Halogenated Aliphatic Hydrocarbon

Physical properties:

Relative molecular mass:	62.4987	
Specific gravity:	0.9106 (20/4)	[85]
	0.9834 (-20/4)	[11]
Boiling point:	-13.80°C	[58]
Melting point:	-153.79°C	[58]
Refractive index:	1.3682	[58]
Vapor pressure:	337.3 kPa @ 20°C	[88]
	77.32 @ -20°C	[80]
Vapor density:	2.15	[63]
Evaporation rate:	NA	
Relative permittivity:	6.26 @ 17.2°C (under pressure)	[11]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	NA	
Electrical resistivity:	NA	
Critical temperature:	156.2°C	[11]
Critical pressure:	5.6 MPa	[11]
Dynamic viscosity:	0.328 mPa-s @ -40°C	
(calculated from	0.298 @ -30°C	
kinematic visc.)	0.273 @ -20°C	
	0.252 @ -10°C	
Kinematic viscosity:	0.3339 $\mu m^2/s$ @ -40°C	[11]
	0.3026 @ -30°C	[11]
	0.2780 @ -20°C	[11]
	0.2563 @ -10°C	[11]
Surface tension:	23.87 mN/m @ -30°C	[11]
	22.27 @ -20°C	[11]
	20.88 @ -10°C	[11]
	16 @ 25°C	[86]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	NA	
Compressibility:	NA	
Electric dipole moment:	NA	
Ionization potential:	9.996 eV (S,PI)	[85]
Volume susceptibility:	-6.64×10^{-6} SI unit (liq @ 15°C)	[85]
Speed of Sound:	NA	
Heat of melting:	4.747 kJ/mol	[11]
Heat of vaporization:	20.811 kJ/mol	[11]
Heat of sublimation:	NA	
Heat capacity @ 17°C:	NA (liq)	
	0.08983 kJ/(mol-K) (gas)	[58]

Heat of combustion:	-1249.8	kJ/mol @ 25°C (liq)	[58]
Heat of formation:	14.6	kJ/mol @ 25°C (liq)	[58]
	33.77	(gas)	[58]
Heat of polymerization:	-105.6	kJ/mol	[86]
Gibbs (free) energy:	51.54	kJ/mol @ 25°C (gas)	[8]

Analytical Chemistry: NA

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Slightly soluble in water; soluble in ethanol, carbon tetrachloride, benzene; very soluble in ether. (0.00011g/100g water @ 25°C [80]; 0.11g water/100g vinyl chloride @ 25°C [11]; 0.27g/100g water @ 25°C [58]).

Form: Colorless gas or liquid; faintly sweet odor; polymerizes in presence of air sunlight, heat or catalyst. Phenol added as polymerization inhibitor when high temperatures are expected.

Use: In the plastics industry; as refrigerant; in organic syntheses; polyvinyl chloride and copolymers; adhesives for plastics. 19th highest volume chemical produced in U.S. (1979).

Fire and Explosion Hazard: Very high.
Flash point: -78°C (CC) [88]; -78.9°C (OC) [86]
lel: 3.6%; uel: 22.0% [63]
Autoign. temp.: 472°C [63]
Extremely flammable gas. 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 carbon monoxide. 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 or CO_2.

Incompatible: With air.

Handling: Keep away from heat, flame, sources of ignition and air. Before storing or handling this material,instructions for its use should be obtained from the supplier. Contact with the skin or by inhalation is prohibited. Prevent skin contact (PVA coated nylon gloves and boots, lab coat, gas-tight goggles). Use in well-ventilated area (fume hood). Organic vapor canister respirator or self-contained breathing apparatus required. Monitoring program is required for all vinyl chloride operations.

Health effects: Irritant to eyes, skin and mucous membranes. In high concentrations, it acts as an anesthetic. Causes skin burns by rapid evaporation and consequent freezing. 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. Listed as a carcinogen by the EPA.

Toxicity: High.
TWA: 1 ppm;
CL: 5 ppm over any 15 minute period
Odor threshold: 10-260 ppm
Exposure: Dizziness and disorientation may start to occur at 25000 ppm over a 3 min period.
Inhalation:
Non-lethal: 500 ppm/4 yr at int.--Carcinogenic effects

WATER H_2O CAS RN: 7732185

Syn: Dihydrogen oxide.

Chemical formula: H_2O 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	[85]
Vapor pressure:	2.3378 kPa @ 20°C	[85]
Vapor density:	NA	
Evaporation rate:	NA	
Relative permittivity:	87.90 @ 0°C	[85]
	85.90 @ 5°C	[85]
	83.95 @ 10°C	[85]
	82.04 @ 15°C	[85]
	80.18 @ 20°C	[85]
	78.36 @ 25°C	[85]
	76.58 @ 30°C	[85]
	73.15 @ 40°C	[85]
	69.88 @ 50°C	[85]
	66.76 @ 60°C	[85]
	63.78 @ 70°C	[85]
	60.93 @ 80°C	[85]
	58.20 @ 90°C	[85]
	55.58 @ 100°C	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.5552 W/(m-K) @ -3°C	[85]
	0.5744 @ 7°C	[85]
	0.6096 @ 27°C	[85]
	0.611 @ 30°C	[58]
	0.6372 @ 47°C	[85]
	0.6594 @ 67°C	[85]
	0.6804 @ 97°C	[85]
Electrical resistivity	0.303 MOhm-m @ 15°C	[58]
	0.256 @ 18°C	[58]
	0.227 @ 20°C	[58]
	0.170 @ 25°C	[58]
	0.129 @ 30°C	[58]
Critical temperature:	374.1oC	[85]
Critical pressure:	22.12 MPa	[85]

Dynamic viscosity: (kinematic viscosity values the same)	1.787 mPa-s @ 0°C	[85]
	1.307 @ 10°C	[85]
	1.002 @ 20°C	[85]
	0.8904 @ 25°C	[85]
	0.7975 @ 30°C	[85]
	0.6529 @ 40°C	[85]
	0.5468 @ 50°C	[85]
	0.4665 @ 60°C	[85]
	0.4042 @ 70°C	[85]
	0.3547 @ 80°C	[85]
	0.3147 @ 90°C	[85]
	0.2818 @ 100°C	[85]
Surface tension:	75.60 mN/m @ 0°C	[85]
	74.22 @ 10°C	[85]
	72.75 @ 20°C	[85]
	71.97 @ 25°C	[85]
	71.18 @ 30°C	[85]
	69.56 @ 40°C	[85]
	67.91 @ 50°C	[85]
	66.18 @ 60°C	[85]
	64.4 @ 70°C	[85]
	62.6 @ 80°C	[85]
	58.9 @ 100°C	[85]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.00020661 K^{-1} @ 20°C	[58]
	0.00025705 @ 25°C	[58]
	0.00030314 @ 30°C	[58]
Compressibility:	0.501 nPa^{-1} @ 0°C	[85]
	0.478 @ 10°C	[85]
	0.458 @ 20°C	[85]
	0.457 @ 25°C	[85]
	0.446 @ 30°C	[85]
	0.441 @ 40°C	[85]
	0.440 @ 50°C	[85]
	0.443 @ 60°C	[85]
	0.449 @ 70°C	[85]
	0.457 @ 80°C	[85]
	0.468 @ 90°C	[85]
	0.480 @ 100°C	[85]
Vapor diffusivity:	22.0 $\mu m^2/s$ @ 0°C	[80]
Solution diffusivity:	0.21 nm^2/s in glycerol	[80]
Electric dipole moment:	6.17 x 10^{-30} C-m	[85]
Ionization potential:	12.6 eV (PI)	[85]
Volume susceptibility:	-154.7 x 10^{-6} SI units @ 20°C	[85]
Speed of sound:	1496.7 m/s @ 25°C	[85]
Heat of melting:	6.012 kJ/mol	[8]
Heat of vaporization:	40.68 kJ/mol	[8]
Heat of sublimation:	50.982 kJ/mol	[58]
Heat capacity @ 25°C:	0.075342 kJ/(mol-K) (liq)	[8]
	0.03360 (gas)	[8]
Heat of combustion:	NA	

Heat of formation:	-286.02	kJ/mol @ 25°C	(liq)	[8]
	-241.98		(gas)	[8]
Gibbs (free) energy:	-237.34	kJ/mol @ 25°C	(liq)	[8]
	-228.74		(gas)	[8]

Analytical chemistry: pKw =	14.9435	@ 0°C	[85]
	14.5346	@ 10°C	[85]
	14.1669	@ 20°C	[85]
	13.9965	@ 25°C	[85]
	13.883	@ 30°C	[85]
	13.542	@ 40°C	[58]
	13.272	@ 50°C	[58]

Electrochemical data: NA

Clay-organic interaction data: NA

Solubility: Miscible with acetic acid, acetone, 1,4-dioxane, ethanol, methanol, and most ionic organic chemicals.

Form: Clear, colorless liquid; no odor; no taste.

Use: Universal solvent except for non-ionic organic chemicals.

Fire and Explosion Hazard: None.
Not combustible.

Incompatible: 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.

m-XYLENE C_8H_{10} CAS RN: 108383

Syn:1,3-Dimethylbenzene; m-dimethylbenzene; m-methyltoluene; 1,3-xylene; 3-xylene; meta-xylene; m-xylol.

Chemical formula: m-$C_6H_4(CH_3)_2$

Monocyclic Aromatic Hydrocarbon

Physical properties:

Relative molecular mass:	106.1674	
Specific gravity:	0.8642	[85]
Boiling point:	139.1°C	[85]
Melting point:	-47.87°C	[85]
Refractive index:	1.4972	[85]
Vapor pressure:	1.20 kPa @ 20°C	[37]
Vapor density:	3.66	[63]
Evaporation rate:	0.7	[37]
Relative permittivity:	2.374 @ 20°C	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.1362 W/(m-K) @ 0°C	[8]
	0.156 @ 20°C	[52]
	0.1577 @ 25°C	[85]
Electrical resistivity:	1.16 x 10^7 MOhm-m	[58]
Critical temperature:	343.90°C	[58]
Critical pressure:	3.536 MPa	[58]
Dynamic viscosity:	0.806 mPa-s @ 0°C	[85]
	0.650 @ 15°C	[85]
	0.620 @ 20°C	[85]
	0.581 @ 25°C	[58]
	0.497 @ 40°C	[85]
Kinematic viscosity:	0.933 $\mu m^2/s$ @ 0°C	
	0.752 @ 16°C	
	0.717 @ 20°C	
	0.672 @ 25°C	
	0.575 @ 40°C	
Surface tension:	33.438 mN/m @ -20°C	[8]
(calculated)	32.334 @ -10°C	[8]
	31.230 @ 0°C	[8]
	30.126 @ 10°C	[8]
	29.022 @ 20°C	[8]
	27.918 @ 30°C	[8]
	26.814 @ 40°C	[8]
	25.710 @ 50°C	[8]
	24.606 @ 60°C	[8]
	23.502 @ 70°C	[8]
	22.398 @ 80°C	[8]
	21.294 @ 90°C	[8]
	20.190 @ 100°C	[8]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.000981 K^{-1}	[58]

Compressibility:	0.744 nPa^{-1} @ 0°C		[85]
	0.794 @ 10°C		[85]
	0.846 @ 20°C		[85]
	0.8621 @ 25°C		[58]
	0.903 @ 30°C		[85]
	0.963 @ 40°C		[85]
	1.025 @ 50°C		[85]
	1.101 @ 60°C		[85]
	1.177 @ 70°C		[85]
	1.256 @ 80°C		[85]
Vapor diffusivity:	NA		
Solution diffusivity:	NA		
Electric dipole moment:	1.234×10^{-30} C-m		[8]
Ionization potential:	8.58 eV (PI)		[85]
Volume susceptibility:	-7.835×10^{-6} SI units @20°C		[85]
Speed of sound:	NA		
Heat of melting:	11.6 kJ/mol		[8]
Heat of vaporization:	36.4 kJ/mol		[8]
Heat of sublimation:	42.71 kJ/mol		[8]
Heat capacity @ 25°C:	0.1834 kJ/(mol-K)	(liq)	[8]
	0.1277	(gas)	[8]
Heat of combustion:	-4554.90 kJ/mol @ 25°C	(liq)	[20]
	-4597.61	(gas)	[20]
Heat of formation:	-25.46 kJ/mol @ 25°C	(liq)	[8]
	17.258	(gas)	[8]
Gibbs (free) energy:	107.73 kJ/mol @ 25°C	(liq)	[8]
	118.95	(gas)	[8]

Analytical chemistry: pKh = 3.2 @ 0°C in HF [58]

Electrochemical data: [48].

Clay-organic interaction data: 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. [75]

Solubility: Almost insoluble in water; miscible with absolute alcohol, ether, acetone, carbon tetrachloride , petroleum ether, benzene and many other organic solvents. (0.03mg/100g water @ 20°C [37]; 0.0146% in water @ 25°C [58])

Form: Colorless liquid; aromatic odor.

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; aviation gasolines.

Fire and Explosion Hazard: High.
Flash point: 28.9°C (CC) [86]
lel: 1.1%; uel: 6.4% [86]
Autoign. temp.: 530°C [86]
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 foam, CO_2 or dry chemical. Water may be ineffective.

Incompatible: Strong oxidizing agents.

Handling: Keep away from heat, sparks and flame. Use with adequate ventilation (fume hood). Avoid breathing vapors (respirator). Avoid contact with eyes, skin or clothing (nitrile or PVA synthetic latex gloves and boots, safety goggles or face shield, lab coat, apron). Keep container tightly closed. Bond and ground containers when transferring liquid. Store in cool, dry, well-ventilated, flammable liquid storage area.

Health effects: Xylenes are moderately toxic if inhaled, come in contact with the eyes or skin, or if swallowed. 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. Xylenes may be narcotic at high concentrations.

Toxicity: Moderate.
TWA: 100 ppm
STEL: 150 ppm
CL: 200 ppm averaged over 10 min period
Peak: 300 ppm for 30 min duration
Odor threshold: 1-200 ppm
Exposure: Workers exposed to concentrations exceeding 200 ppm complain of anorexia, nausea, vomiting and abdominal pain.

o-XYLENE C_8H_{10} CAS RN: 95476

Syn:1,2-Dimethylbenzene; o-dimethylbenzene; o-methyltoluene; 1,2-xylene; 2-xylene; ortho-xylene; o-xylol.

Chemical formula: $o\text{-}C_6H_4(CH_3)_2$

Monocyclic Aromatic Hydrocarbon

Physical properties:

Relative molecular mass:	106.1674	
Specific gravity:	0.8802	[85]
Boiling point:	144.4°C	[85]
Melting point:	-25.18°C	[85]
Refractive index:	1.5055	[85]
Vapor pressure:	0.933 kPa @ 20°C	[37]
Vapor density:	3.7	[37]
Evaporation rate:	0.7	[37]
Relative permittivity:	2.568 @ 20°C	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	0.1442 W/(m-K) @ 0°C	[8]
	0.156 @ 20°C	[52]
	0.1055 @ 33°C	[8]
	0.1428 @ -20 - 80°C	[85]
Electrical resistivity:	1.5×10^7 MOhm-m	[58]
Critical temperature:	357.18°C	[58]
Critical pressure:	3.734 MPa	[58]
Dynamic viscosity:	1.105 mPa-s @ 0°C	[85]
	0.876 @ 16°C	[85]
	0.820 @ 20°C	[85]
	0.756 @ 25°C	[58]
	0.627 @ 40°C	[85]
Kinematic viscosity:	1.255 $\mu m^2/s$ @ 0°C	
	0.995 @ 16°C	
	0.932 @ 20°C	
	0.859 @ 25°C	
	0.712 @ 40°C	
Surface tension:	34.712 mN/m @ -20°C	[8]
(calculated)	33.611 @ -10°C	[8]
	32.510 @ 0°C	[8]
	31.409 @ 10°C	[8]
	30.308 @ 20°C	[8]
	29.207 @ 30°C	[8]
	28.106 @ 40°C	[8]
	27.005 @ 50°C	[8]
	25.904 @ 60°C	[8]
	24.803 @ 70°C	[8]
	23.702 @ 80°C	[8]
	22.601 @ 90°C	[8]
	21.500 @ 100°C	[8]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.000952 K^{-1}	[58]

Compressibility:	0.8105 nPa^{-1} @ 25°C			[58]
Vapor diffusivity:	NA			
Solution diffusivity:	NA			
Electric dipole moment:	2.07 x 10^{-30} C-m			[85]
Ionization potential:	8.56 eV (PI)			[85]
Volume susceptibility:	-8.093 x 10^{-6} SI units		@20°C	[85]
Speed of sound:	NA			
Heat of melting:	13.6 kJ/mol			[8]
Heat of vaporization:	36.8 kJ/mol			[8]
Heat of sublimation:	43.46 kJ/mol			[8]
Heat capacity @ 25°C:	0.188 kJ/(mol-K)		(liq)	[8]
	0.1333		(gas)	[8]
Heat of combustion:	-4555.91 kJ/mol	@ 25°C	(liq)	[20]
	-4599.37		(gas)	[20]
Heat of formation:	-24.451 kJ/mol	@ 25°C	(liq)	[8]
	19.008		(gas)	[8]
Gibbs (free) energy:	110.4 kJ/mol	@ 25°C	(liq)	[8]
	122.2		(gas)	[8]

Analytical chemistry: NA

Electrochemical data: [48].

Clay-organic interaction data: 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. [75]

Solubility: Almost insoluble in water; miscible with absolute alcohol, ether, acetone, carbon tetrachloride, petroleum ether, benzene and many other organic solvents. (0.03mg/100g water @ 20°C [37]; 0.0175% in water @ 25°C [58])

Form: Colorless liquid; aromatic odor.

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; aviation gasolines.

Fire and Explosion Hazard: High.
Flash point: 17.2°C (CC); 23.9°C (OC) [86]
lel: 1.1%; uel: 7.0% [86]
Autoign. temp.: 465°C [86]
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 foam, CO_2 or dry chemical. Water may be ineffective.

Incompatible: Strong oxidizing agents.

Handling: Keep away from heat, sparks and flame. Use with adequate ventilation (fume hood). Avoid breathing vapors (respirator). Avoid contact with eyes, skin or clothing (nitrile or PVA synthetic latex gloves and boots, safety goggles or face shield, lab coat, apron). Keep container tightly closed. Bond and ground containers when transferring liquid. Store in cool, dry, well-ventilated, flammable liquid storage area.

Health effects: Xylenes are moderately toxic if inhaled, come in contact with the eyes or skin, or if swallowed. 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. Xylenes may be narcotic at high concentrations.

Toxicity: Moderate.
TWA: 100 ppm
STEL: 150 ppm
CL: 200 ppm averaged over 10 min period
Peak: 300 ppm for 30 min duration
Odor threshold: 1-200 ppm
Exposure: Workers exposed to concentrations exceeding 200 ppm complain of anorexia, nausea, vomiting and abdominal pain.

p-XYLENE C_8H_{10} CAS RN: 106423

Syn:1,4-Dimethylbenzene; p-dimethylbenzene; p-methyltoluene; 1,4-xylene; 4-xylene; para-xylene; p-xylol.

Chemical formula: $p\text{-}C_6H_4(CH_3)_2$

Monocyclic Aromatic Hydrocarbon

Physical properties:

Relative molecular mass:	106.1674	
Specific gravity:	0.8611	[85]
Boiling point:	138.35°C	[85]
Melting point:	13.26°C	[85]
Refractive index:	1.4958	[85]
Vapor pressure:	1.20 kPa @ 20°C	[37]
Vapor density:	3.66	[63]
Evaporation rate:	0.7	[37]
Relative permittivity:	2.27 @ 20°C	[85]
Loss tangent:	NA	
Relaxation time:	NA	
Thermal conductivity:	NA	
Electrical resistivity:	1.3×10^7 MOhm-m	[58]
Critical temperature:	343.08°C	[58]
Critical pressure:	3.511 MPa	[58]
Dynamic viscosity:	0.644 mPa-s @ 20°C	[58]
	0.605 @ 25°C	[58]
	0.566 @ 30°C	[58]
	0.513 @ 40°C	[85]
Kinematic viscosity:	0.748 $\mu m^2/s$ @ 20°C	
	0.703 @ 25°C	
	0.657 @ 30°C	
	0.596 @ 40°C	
Surface tension:	29.079 mN/m @ 15°C	[8]
(calculated)	28.542 @ 20°C	[8]
	27.468 @ 30°C	[8]
	26.394 @ 40°C	[8]
	25.320 @ 50°C	[8]
	24.246 @ 60°C	[8]
	23.172 @ 70°C	[8]
	22.098 @ 80°C	[8]
	21.024 @ 90°C	[8]
	19.950 @ 100°C	[8]
Contact angle:	NA on quartz	
	NA on calcite	
	NA on silica	
Thermal expansion coef.:	0.000956 K^{-1}	[58]
Compressibility:	0.8588 nPa^{-1} @ 25°C	[58]
Vapor diffusivity:	NA	
Solution diffusivity:	NA	
Electric dipole moment:	0	[85]
Ionization potential:	8.44 eV (PI)	[85]
Volume susceptibility:	-7.824×10^{-6} SI units @20°C	[85]
Speed of sound:	NA	
Heat of melting:	17.1 kJ/mol	[8]

Heat of vaporization:	36.0 kJ/mol		[8]
Heat of sublimation:	42.41 kJ/mol		[8]
Heat capacity @ 25°C:	0.1825 kJ/(mol-K)	(liq)	[85]
	0.1269	(gas)	[85]
Heat of combustion:	-4555.91 kJ/mol @ 25°C	(liq)	[20]
	-4598.32	(gas)	[20]
Heat of formation:	-24.37 kJ/mol @ 25°C	(liq)	[20]
	18.00	(gas)	[20]
Gibbs (free) energy:	NA		

Analytical chemistry: pKh = 5.7 @ 0°C in HF [58]

Electrochemical data: [48].

Clay-organic interaction data: 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. [75]

Solubility: Almost insoluble in water; miscible with absolute alcohol, ether, acetone, carbon tetrachloride, petroleum ether, benzene and many other organic solvents. (0.03mg/100g water @ 20°C [37]; 0.0156% in water @ 25°C [58])

Form: Colorless liquid (plates or prisms at low temperatures); aromatic odor.

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; aviation gasolines.

Fire and Explosion Hazard: High.
Flash point: 27.2°C (CC) [86]
lel: 1.1%; uel: 6.6% [86]
Autoign. temp.: 465°C [86]
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 foam, CO_2 or dry chemical. Water may be ineffective.

Incompatible: Strong oxidizing agents.

Handling: Keep away from heat, sparks and flame. Use with adequate ventilation (fume hood). Avoid breathing vapors (respirator). Avoid contact with eyes, skin or clothing (nitrile or PVA synthetic latex gloves and boots, safety goggles or face shield, lab coat, apron). Keep container tightly closed. Bond and ground containers when transferring liquid. Store in cool, dry, well-ventilated, flammable liquid storage area.

Health effects: Xylenes are moderately toxic if inhaled, come in contact with the eyes or skin, or if swallowed. 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. Xylenes may be narcotic at high concentrations.

Toxicity: Moderate.
TWA: 100 ppm
STEL: 150 ppm
CL: 200 ppm averaged over 10 min period
Peak: 300 ppm for 30 min duration
Odor threshold: 1-200 ppm
Exposure: Workers exposed to concentrations exceeding 200 ppm complain of anorexia, nausea, vomiting and abdominal pain.

REFERENCES AND BIBLIOGRAPHY

[1] ASTM Committee on Terminology, 1979, Compilation of ASTM Standard Definitions, 4th ed.: Philadelphia, PA, American Society for Testing and Materials, 700 p.

[2] Anderson, J.T. and Stocker, J.H., 1983, Oxidative coupling: in Organic Electrochemistry, 2nd ed., M.M. Baizer and H. Lund, eds., NY, Marcel Decker, p. 691-726.

[3] Bagotsky, V.S. and Vasilyev, Yu.B., 1966, Oxidation reactions of organic compounds on platinum electrodes: Electrochimica Acta, v. 9., p. 869-882.

[4] Baizer, M.M., 1983, Electrolytic reductive coupling: in Organic Electrochemistry, 2nd ed., M.M. Baizer and H. Lund, eds., NY, Marcel Decker, Inc., p. 639-689.

[5] Baker, J.T., Chemical Co., 1986, Material Safety Data Sheets: Phillipsburg, NJ, various pagination.

[6] Bretherick, L., 1981, Hazards in the Chemical Laboratory, 3rd ed.: The Royal Society of Chemistry, London, 567 p.

[7] Cover, E.E. and Folliard, J.T., 1971, Elucidation of electrochemical mechanisms using the vibrating dropping mercury electrode. Noncatalytic waves of quinine, quinoline and 3-aminoquinoline: J. Electroanal. Chem. Interfacial Electrochem., v. 30, p. 143-159.

[8] Dean, J.A., ed., 1985, Lange's Handbook of Chemistry, 13th ed.: NY, McGraw-Hill Book Co., various pagination.

[9] Drazil, J.V., 1983, Quantities and Units of Measurements--A Dictionary and Handbook: London, Mansell Publishing Ltd., 313 p.

[10] Dreisbach, R.R., 1955, Physical Properties of Chemical Compounds-I: Washington, D.C., American Chemical Society, 536 p.

[11] Dreisbach, R.R., 1959, Physical Properties of Chemical Compounds-II: Washington, D.C., American Chemical Society, 491 p.

[12] Dreisbach, R.R., 1961, Physical Properties of Chemical Compounds-III: Washington, D.C., American Chemical Society, 489 p.

[13] Eberson, L. and Utley, J.H.P., 1983, Anodic oxidation: in Organic Electrochemistry, 2nd ed., M.M. Baizer and H. Lund, eds., NY, Marcel decker, p. 775-804.

[14] Fairhall, L.T., 1957, Industrial Toxicology, 2nd ed.: Baltimore, MD, Williams and Wilkins, 376 p.

[15] Feoktistov, L.G., 1983, Saturated carbonyl compounds and derivatives: in Organic Electrochemistry, 2nd ed., M.M. Baizer and H. Lund, eds., NY, Marcel Decker, p. 315-358.

[16] Finkel, A.J., 1983, Hamilton and Hardy's Industrial Toxicology, 4th ed.: John Wright-PSG Inc., 428 p.

[17] Folliard, J.T. and Cover, R.E., 1971, Elucidation of electrochemical mechanisms using the vibration dropping mercury electrode. Catalytic waves of quinine, quinoline and 3-aminoquinoline: J. Electroanal. Chem. Interfacial Electrochem., v. 33, p. 463-472.

[18] Fujinaga, T., Izutsu, K. and Takaoka, K., 1966, Polarographic reduction of quinoline and its derivatives in non-aqueous solvents: J. Electroanalytical Chemistry, v. 12, p. 203-215.

[19] Given, P.H. and Peover, M.E., 1960,Polarographic reduction of aromatic hydrocarbons and carbonyl compounds in dimethylformamide in the presence of proton donors: J. Chemical Society [London], v. 60B, p. 385-393.

[20] Gray, D.E., coord. ed., 1972, American Institute of Physics Handbook, 3rd ed.: NY, McGraw-Hill Book Co., various pagination.

[21] Greenland, D.J. and Hayes, M.H.B., 1981, The Chemistry of Soil Processes: NY, John Wiley & Sons, 714 p.

[22] Hammerich, O., 1983, Anodic oxidation of oxygen containing compounds: in Organic Electrochemistry, 2nd ed., M.M. Baizer and H. Lund, eds., NY, Marcel Decker, p.485-517.

[23] Hansen, R.L., Toren, P.E. and Young, P.E., 1964, Nitro-p-terphenyls. II. The relation between charge-transfer properties and polarographic oxidation and reduction potentials: J. Physical Chemistry, v. 70, p. 1653-1657.

[24] Hawley, G.G., 1981, The Condensed Chemical Dictionary, 10th ed.: NY, Van Nostrand Reinhold Co., 1135 p.

[25] Heyrovsky, M., 1962, Oscillopolarographic behavior of ketones in alkali medium: Chemicke Zvesti, v. 16, p. 338-341.

[26] Hibbert, D.B. and James, A.M., 1984, Dictionary of Electrochemistry, 2nd ed.: NY, John Wiley & Sons, 308 p.

[27] Hodgman, C.D., ed.-in-chief, 1960, Tables for Identification of Organic Compounds--Supplement to Handbook of Chemistry and Physics: Cleveland, OH, CRC Press, 241 p.

[28] Jacobs, M.B., 1941, The Analytical Chemistry of Industrial Poisons, Hazards, and Solvents: NY, Interscience Publishers, Inc., 661 p.

[29] Karapet'yants, M.Kh. and Karapet'yants, M.L., 1970, Thermodynamic Constants of Inorganic and Organic Compounds: NY, John Wiley & Sons, Inc., 461 p.

[30] Klemm, L.H. and Kohlik, A.J., 1963, Polarographic reductions of some alkyl-, alkylene- and polymethylnaphthalenes: J. Organic Chemistry, v. 28, p. 2044-2049.

[31] Klemm, L.H., Lind, C.D. and Spence, J.T., 1960, Polarographic reduction of some biaryls and arylalkenes: J. Organic Chemistry, v. 25, p. 611-616.

[32] Klemm, L.H., Solomon, W.C. and Kohlik, A.J., 1962, Coplanarity effects on the spectral, gas chromatographic, polarographic, and Diels-Alder characteristics of 1-alkyl-1-(2-naphthyl)ethenes: J. Organic Chemistry, v. 27, p. 2777-2786.

[33] Kolthoff, I.M. and Reddy, T.B., 1961, Polarography and voltammetry in dimethyl sulfoxide: J.Electrochemical Society, v. 108, p. 980-985.

[34] Lezhneva, N.A. and Kruglov, E.A., 1965, Polarographic determination of bicyclic aromatic hydrocarbons in petroleum products: Chemistry and Technology of Fuels and Oils [USSR], v. 10, p. 890-894.

[35] Loveland, J.W. and Dimeler, G.R., 1961, Anodic voltammetry to +2.0 volts. Application to hydrocarbons and oxidation stability studies: Analytical Chemistry, v. 33, p. 1196-1201.

[36] Lund, H., 1983, Use of the solvated electron: in Organic Electrochemistry, 2nd ed., M.M. Baizer and H. Lund, eds., NY, Marcel Decker, Inc., p. 873-885.

[37] Mackison, F.W., Stricoff, R.S. and Partridge, L.J., Jr., eds., 1981, Occupational Health Guidelines for Chemical Hazards: U.S. Dept. Health and Human Services, Nat. Inst. Occupational Safety and Health, DHHS (NIOSH) Pub. No. 81-123, various pagination.

[38] Mather, W.B., Jr., 1961, Chronopotentiometry in acetic acid anhydride. Oxidation and reduction of the solvent: Analytical Chemistry, v. 33, p. 1634-1637.

[39] May, J., 1966, Solvent odor thresholds for the evaluation of solvent odors in the atmosphere: Staub-Reihhalt, v. 26, p. 385-389.

[40] Meidl, J.H., 1970, Explosive and Toxic Hazardous Materials: Beverly Hills, CA, Glencoe Press, 387 p.

[41] Meites, L., Zuman, P. and Rupp, E.B., 1977, CRC Handbook Series in Organic Electrochemistry, Volume VI: Cleveland, OH, CRC Press, Inc., 538 p.

[42] Meites, L., Zuman, P. and Rupp, E.B., 1977, CRC Handbook Series in Organic Electrochemistry: Cleveland, OH, CRC Press, 6 Volumes.

[43] Meyer, E., 1977, Chemistry of Hazardous Materials: Englewood Cliffs, NJ, Prentice-Hall, Inc., 370 p.

[44] Moore, J.W. and Ramonmoorthy, S., 1984, Organic Chemicals in Natural Water--Applied monitoring and impact assessment: NY, Springer-Verlag, 289 p.

[45] NIOSH, 1985, Pocket Guide to Chemical Hazards: U.S. Dept. Health and Human Services, Public Health Service, Center for Disease Control, Nat. Inst. Occupational Safety and Health, DHEW (NIOSH) Pub. No. 78-210, 5th printing, various pagination.

[46] National Fire Protection Association (NFPA), 1981, Fire Protection Guide on Hazardous Materials, 4th ed., Nos. 325A, 325M, 49, 491M and 704M: Boston, MA, various pagination.

[47] National Research Council, 1981, Prudent Practices for Handling Hazardous Chemicals in Laboratories: Commission on Hazardous Substances in the Laboratory, Assembly of Mathematical and Physical Sciences, NRC, National Academy Press, 291 p.

[48] Neikam, W.C. and Desmond, M.M., 1964, A molecular orbital study of polarographic oxidation potentials of methyl substituted aromatic hydrocarbons: J. American Chemical Society, v. 86, p. 4811-4814.

[49] Neikam, W.C., Dimeler, G.R. and Desmond, M.M., 1964, Correlation of electrochemical oxidation potential of organic compounds with photoionization potential: J. Electrochemical Society, v. 111, p. 1190-1192.

[50] Office of the Federal Register, National Archives and Records Administration, 1986, Code of Federal Regulations, Title 40, Parts 100 to 149.

[51] Osa, T. and Kuwana, T., 1969, Nonaqueous electrochemistry using optically transparent electrodes: J. Electroanal. Chem. Interfacial Electrochem., v. 22, p. 389-406.

[52] Perry, R.H. and Chilton, C.H., eds., 1973, Chemical Engineer's Handbook, 5th ed.: NY, McGraw-Hill Book Co., various pagination.

[53] Peterson, D., 1979, The OSHA Compliance Manual, Revised Edition: NY, McGraw-Hill Book Co., 241 p.

[54] Plumb, R.H., Jr. and Pitchford, A.M., 1985, Volatile organic scans--Implications for ground water monitoring: in Proc. of the API and NWA Conf. on Petroleum Hydrocarbons and Organic Chemicals in Ground Water-Prevention, Detection and Restoration, 11/13-15/85, Houston, TX, p. 207-222.

[55] Proctor, N.H. and Hughes, J.P., 1978, Chemical Hazards in the Workplace: Philadelphia, PA, Lippincott, 533 p.

[56] Pungor, E. and Szepesvary, E., 1968, Voltammetric studies with silicone rubber-based graphite electrodes: Analytica Chimica Acta, v. 43, p. 289-296.

[57] Pysh, E.S. and Yang, N.C., 1963, Polarographic oxidation potentials of aromatic compounds: J. American Chemical Society, v. 85, p. 2124-2130.

[58] Riddick, J.A., Bunger, W.B. and Sakano, T.K., 1986, Organic Solvents. Physical Properties and Methods of Purification, 4th ed.: NY, John Wiley & Sons, 1325 p.

[59] Rieke, R.D., Rich, W.E. and Ridgway, T.H., 1971, Ring strain effects. III. Reduction and oxidation potential shifts: J. American Chemical Society, v. 93, p. 1962-1967.

[60] Rodgers, R.D. and McFarlane, J.C., 1982, Sorption of carbon tetrachloride, ethylene dibromide and trichloroethylene on soil and clay: (U.S. EPA) Environmental Monitoring and Support Lab., Las Vegas, NV, Report No. EPA-600/J-81-560, NTIS PB82-224 361, 9 p., Environmental Monitoring and Assessment, V.1, p. 155-162.

[61] Ryvolova, A., 1963, The mechanisms of the polarographic reduction of phthalic acid diester in alkaline solution: Collection of Czechoslovak Chemical Communications, v. 28, p. 1985-1992.

[62] Sasaki, K., Urata, H., Uneyama, K. and Nagaura, S., 1967, Anodic methoxylation of alkylbenzenes: Electrochimica Acta, v. 12, p. 137-146.

[63] Sax, N.I., 1984, Dangerous Properties of Industrial Materials, 6th ed.: NY, Van Nostrand Reinhold, 3124 p.

[64] Scheiler, L. and Pauze, D., 1976, Hazardous Materials: NY, Van Nostrand Reinhold Co., 249 p.

[65] Sease, J.W., Burton, F.G. and Nichol, S.L., 1968, On the mechanisms of the electrolytic reduction of the carbon-halogen bond. II. A rho-sigma study: J. American Chemical Society, v. 90, p. 2595-2598.

[66] Shriver, D.F., Smith, D.E. and Smith, P., 1964, Reduction potentials and electronic structure of phenyl-substituted borazines: J. American Chemical Society, v. 86, p. 5153-5160.

[67] Shugar, G.J., Shugar, R.A., Bauman, L. and Bauman, R.S., 1981, Chemical Technician's Ready Reference Handbook, 2nd ed.: NY, McGraw-Hill Book Co., 867 p.

[68] Simonet, J., 1983, Electrogenerated reagents: in Organic Electrochemistry, 2nd ed., M.M. Baizer and H. Lund, eds., NY, Marcel Decker, p. 843-871.

Sittig, M., 1985, Handbook of Toxic and Hazardous Chemicals and Carcinogens, 2nd ed.: Park Ridge, NJ, Noyes Publications, 950 p.

[70] Spritzer, M.S., Costa, J.M. and Elving, P.J., 1965, Polarographic reduction of pyridium ion in pyridine. Application to the determination of Bronsted and Lewis acids: Analytical Chemistry, v. 37, p. 211-217.

[71] Steere, N.V., 1967, CRC Handbook of Laboratory Safety: Cleveland, OH, The Chemical Rubber Co., 568 p.

[72] Sternberg, H.W., Markby, R. and Wender, I., 1963, Electrochemical reduction of the benzene ring: J. Electrochemical Society, v. 110, p. 425-429.

[73] Strauss, H.J. and Kaufman, M., 1976, Handbook for Chemical Technicians: NY, McGraw-Hill Book Co., various pagination.

[74] Suatoni, J.C., Snyder, R.E. and Clark, R.O., 1961, Voltammetric studies of phenol and aniline ring substitution: Analytical Chemistry, v. 33, p. 1894-1897.

[75] Theng, B.K.G., 1974, The Chemistry of Clay-Organic Reactions: NY, John Wiley & Sons, 343 p.

[76] Thurman, E.M., 1986, Organic Geochemistry of Natural Waters: Boston, MA, Martinus Nijhoff/Dr. W. Junk Publishers, 497 p.

[77] Tsuji, K. and Elving, P.J., 1969, Polarographic measurements of relative strengths of Bronsted acids in pyridine. Dispersion and solvation effects in acid-base equilibria. Analysis of Bronsted acid mixtures: Analytical Chemistry, v. 41, p. 286-294.

[78] Turner, R. and Elving, P.J., 1965, Electroxidation in pyridine at pyrolytic graphite electrode: Analytical Chemistry, v. 37, p. 467-469.

[79] U.S. Office of Technology Assessment, Wash., DC, 1984, Protecting the Nation's Ground water from Contamination: 2 volumes, various pagination.

[80] Verschueren, K., 1983, Handbook of Environmental Data on Organic Chemicals: NY, Van Nostrand Reinhold Co., 1296 p.

[81] Washburn, E.W., ed.-in-chief, 1929, International Critical Tables of Numerical Data, Physics, Chemistry and Technology, Volume VI: National Research Council, NY, McGraw-Hill Book Co., Inc., 471 p.

[82] Wawzonek, S and Wagenknecht, J.H., 1963, Polarographic studies in acetonitrile and dimethylformamide. VII. The formation of benzene: J. Electrochemical Society, v. 110, p. 420-422.

[83] Wawzonek, S. and Duty, R.C., 1961, Polarographic studies in acetonitrile and dimethylformamide. VI. The formation of dihalocarbenes: J. Electrochemical Society, v. 108, p. 1135-1138.

[84] Weast, R.C. and Astle, M.J., 1985, CRC Handbook of Data on Organic Compounds: Cleveland, OH, CRC Press, 2 Volumes.

[85] Weast, R.C., ed.-in-chief, 1985, CRC Handbook of Chemistry and Physics, 66th ed.: Cleveland, OH, CRC Press, various pagination.

[86] Weiss, G., ed., 1986, Hazardous Chemicals Data Book, 2nd ed.: Park Ridge, NJ, Noyes Data Corp., 1069 p.

[87] Wiberg, K.B. and Lewis, T.P., 1970, Polarographic reduction of the azines: J. American Chemical Society, v. 92, p. 7154-7160.

[88] Windholz, M., 1983, The Merck Index--An Encyclopedia of Chemicals, Drugs, and Biologicals, 10th ed.: Merck & Co., various pagination.

[89] Yariv, S. and Cross, H., 1979, Geochemistry of Colloid Systems for Earth Scientist: NY, Springer-Verlag, 450 p.

[90] Zabetakis, M.G., 1965, Flammability Characteristics of Combustible Gases and Vapors: U.S. Bureau of Mines Bulletin 627, 121 p.

[91] Zachara, J.M., Ainsworth, C.C., Felice, L.J. and Resch, C.T., 1986, Quinoline sorption to subsurface materials: Role of pH and retention of the organic cation: Environmental Science and Technology, v. 20, p. 620-627.