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THERMODYNAMIC PROPERTIES OF MINERALS

By Richard A. Robie

UNITED STATES DEPARTMENT OF THE INTERIOR

GEOLOGICAL SURVEY

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Report TEI-816

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In the ten years since the publication of the National Bureau of Standards comprehensive tables of thermochemical properties, by Rossini and others (1952), a very large body of modern calorimetric and equilibrium data has become available. Because of the complex interrelations among many thermochemical data and the necessity for internal consistency among these values, a complete revision of this standard reference is required. This is also true of the summaries of thermochemical data for the sulfides (Richardson and Jeffes 1952) and for the oxides (Coughlin 1954).

The following tables present critically selected values for the heat and free energy of formation, the logarithm of the equilibrium constant of formation Log K_f, the entropy and the molar volume, at 298.15°K (25.0°C) and one atmosphere for minerals.

Except for the gases, the molar volumes were taken directly from section of this handbook. For a gas, the standard state is the ideal gas at one atmosphere pressure, and consequently all ideal gases have the same molar volume, equal to RT, at a given temperature. The values of the molar volume given in section are those for the real gas at 298.15°K and one atmosphere and are therefore different from those given here.

For all compounds except the silicates, the heat and free energy and Log K_f refer to formation from the elements in their standard states. Thermodynamic properties of elements not listed in these tables but used in the calculations were taken from Kelley and King (1961) and Stull and Sinke (1956).

For the silicates $\Delta H^\circ_{f,298.15}$, $\Delta F^\circ_{f,298.15}$ and Log K_f refer to formation from the oxides in their standard states. This practice was adopted to conform to the more common usage by petrologists and

mineralogists, and to correspond with the most commonly measured quantity. Data are given for most oxides so that the conversion to elements as reference states may be carried out for most silicates. Values of ΔH_f° or ΔF_f° for K_2O and Na_2O have not been included because of the large uncertainties in these quantities.

The standard state adopted for sulfur is the orthorhombic solid. Data have been included, however, for $\Delta H^\circ_{f,\,298.15}$, $\Delta F^\circ_{f,\,298.15}$ and $S^\circ_{298.15}$ for diatomic sulfur, that is for the reaction

$$2\,S_{rhomb} \longleftrightarrow S_2\ gas$$

for those who prefer to use S_2 as a reference state in calculations involving sulfides.

Specific heat data at higher temperatures have not been included because of the ready availability of Kelley's (1960) excellent modern summary of such data.

Tables of the change in free energy with pressure at high temperatures were calculated for H_2O and CO_2 from modern PVT data and are here included. These data may also be used to obtain the fugacity of H_2O or CO_2 using the relation:

$$\ln \frac{f}{f^\circ} = \frac{F_{P,T} - F^\circ_T}{RT}$$

and where f° is the fugacity of the ideal gas at one atmosphere pressure. Complete thermodynamic functions at high temperatures in the ideal gas state, at one atmosphere, (the standard state for gases) are also given for H_2O, CO_2, and S_2.

The unit of energy is the defined calorie, equal to 4.1840 absolute joules. Zero degrees celsius is taken as 273.15°K in accordance with the 1954 definition of the thermodynamic temperature scale (Cohen, Crowe

and DuMond, 1957). These authors' values for the basic physical constants, converted to the chemical scale of atomic weights, were also adopted. The formula weights are based on the International Atomic Weights for 1957 (Wichers, 1958). Symbols and constants used in these tables are given in table 1.

Table 1

T	=	Temperature in degrees Kelvin.
gfw	=	Gram formula weight.
S_T	=	Entropy at temperature T in cal/deg gfw.
ΔH_f	=	Heat of formation from reference state in cal/gfw.
ΔF_f	=	Free energy of formation from reference state in cal/gfw.
molar volume	=	Volume in cm^3 of one gram formula weight at one atmosphere and 298.15°K.
°	=	Superscript indicates the substance is in its standard state.
R	=	Gas constant, 1.98726 ±.00008 cal/deg gfw (mole). 8.31469 ±.00032 joules/deg gfw (mole).
calorie	=	Unit of energy, 4.1840 absolute joules. 41.2929 cm^3 atmosphere.
A	=	Avogadro's number, (6.02322 ±.00016) x 10^{23} molecules/gfw (mole).
f	=	Fugacity in atmospheres.
P	=	Pressure, in atmospheres or bars.
Atm	=	Atmosphere, 1,013,250 dynes/cm^2.
bar	=	Bar, 1,000,000 dynes/cm^2.
log	=	Logarithm to the base 10.
ln	=	Logarithm to the base e = 2.71828...

Cohen, Crowe and DuMond, Fundamental Constants of Physics, Interscience Pub., New York, 1957.

Wichers, J. Am. Chem. Soc. 80, 4121, 1958.

For more extensive summaries of thermochemical data, the reader is referred to the works cited below.

Rossini and others, U. S. Nat. Bur. Stds., Cir. 500, 1952.

Richardson and Jeffes, J. Iron and Steel Inst. 171, 167, 1952.

Coughlin, U. S. Bur. Mines Bull. 542, 1954.

Stull and Sinke, Advances in Chem. 19, Am. Chem. Soc., 1956.

Kelley, U. S. Bur. Mines Bull. 584, 1960.

Kelley and King, U. S. Bur Mines Bull. 592, 1961.

Hilsenrath and others, U. S. Nat. Bur. Stds. Cir. 564, 1955.

JANAF Interim Thermochemical Tables, the Dow Chemical Company, Midland, Mich., 1960-1962.

ELEMENTS

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
Ag	Silver	107.880	10.274 ±.005	10.20 ±.05	1	0	0		
Au	Gold	197.0	10.216 ±.005	11.32 ±.02	1	0	0		
C	Diamond	12.011	3.4167 ±.0005	0.566 ±.003	2, 3	453 ±5	693 ±15	-0.508	4
C	Graphite	12.011	5.299 ±.002	1.372 ±.005	5	0	0		
Cu	Copper	63.54	7.114 ±.004	7.95 ±.03	1, 6	0	0		
Fe	α-Iron	55.85	7.093 ±.004	6.49 ±.03	1	0	0		
Ni	Nickel	58.71	6.589 ±.005	7.14 ±.02	1	0	0		
Pt	Platinum	195.09	9.092 ±.005	9.95 ±.05	1	0	0		
S	α-Sulfur	32.066	15.53 ±.02	7.62 ±.04	1	0	0		
S	β-Sulfur	32.066		7.78 ±.06	1	70 ±20	15 ±10	-.011	7
S_2	Ideal Gas	64.132	24466.1 ±1.0	54.51 ±.10	8	30840 ±200	19138 ±200	-14.028	8
Pb	Lead	207.21	18.269 ±.005	15.49 ±.05	1	0	0		
Sn	β-Tin	118.70	16.290 ±.010	12.29 ±.06	1	0	0		

ELEMENTS (continued)

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
Sb	Antimony	121.76	18.18 ±.02	10.92 ±.06	1	0	0		
As	Arsenic	74.91	12.96 ±.05	8.36 ±.20	1	0	0		
Bi	Bismuth	209.00	21.311 ±.010	13.50 ±.20	1	0	0		
Zn	Zinc	65.38	9.164 ±.005	9.95 ±.05	1	0	0		
Se	Selenium	78.96	16.42 ±.02	10.14 ±.05	1	0	0		
Te	Tellurium	127.61	20.48 ±.02	11.88 ±.10	1	0	0		
O_2	Oxygen (ideal gas)	32.00	24466.1 ±1.0	49.01 ±.01	1	0	0		
Cl_2	Chlorine (ideal gas)	70.914	24466.1 ±1.0	53.29 ±.01	1	0	0		
Si	Silicon	28.09	12.058 ±.006	4.497 ±.009	87	0	0		

HALIDES

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
NaCl	Halite	58.448	27.018 ±.007	17.33 ±.10	1	-98230 ±300	-91812 ±350	67.30	4
KCl	Sylvite	74.557	37.528 ±.007	19.70 ±.05	1	-104180 ±200	-97521 ±250	71.48	4
NaF	Villiaumite	41.991	14.99 ±.01	12.26 ±.07	1	-136300 ±300	-129092 ±350	94.62	9
AgBr	Bromyrite	187.796	28.99 ±.01	25.60 ±.10	1	-23742 ±200	-22930 ±200	16.81	4
AgCl	Ceragyrite	143.337	25.73 ±.01	23.00 ±.10	1	-30348 ±250	-26220 ±200	19.22	4
AgI	Iodyrite	234.79	41.31 ±.02	27.60 ±.40	1	-14821 ±350	-15850 ±300	11.62	4
CaF_2	Fluorite	78.08	24.54 ±.01	16.46 ±.08	1	-290300 ±400	-277796 ±450	20.36	4
MgF_2	Sellaite	62.32	19.64 ±.02	13.68 ±.07	1	-263500 ±300	-250805 ±350	183.84	4
HgCl	Calomel	236.067	32.94 ±.02	23.08 ±.30	1	-31660 ±300	-25175 ±200	18.45	4
Na_3AlF_6	Cryolite	209.953	70.86 ±.25	56.98 ±.40	1	-784700 ±900	-745413 ±1000	546.38	9
$MgCl_2$	Chloromagnesite	95.234	41.05 ±.15	21.42 ±.20	1	-153400 ±400	-141570 ±450	103.76	4
HCl	Ideal Gas	36.465	24466.1 ±1.0	44.64_5 ±.05	8	-21970 ±150	-22684 ±180	16.63	8
$MnCl_2$	Sacchite	125.854		28.26 ±.05	89	-115190 ±120	-105446 ±300	77.290	90

OXIDES AND HYDROXIDES

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
Al_2O_3	Corundum	101.96	25.57 ±.01	12.18 ±.03	1	-400400 ±300	-378073 ±330	277.12	10
AlO(OH)	Boehmite	59.988	19.54 ±.02	11.58 ±.05	1	-235500 ±3500	-217670 ±3500	159.55	4
$HAlO_2$	Diaspore	59.988	17.76 ±.03	8.43 ±.04	1				
$Al(OH)_3$	Gibbsite	78.004	31.96 ±.04	16.75 ±.10	1	-306380 ±300	-273480 ±350	200.46	11
As_2O_3	Arsenolite	197.82	51.12 ±.03	25.6 ±.5	1	-157000 ±400	-129170 ±500	94.68	12
BeO	Bromellite	25.013	8.315 ±.005	3.37 ±.02	1	-143100 ±150	-136118 ±200	99.77	12
Bi_2O_3	Bismite	466.00		36.2 ±.6	1	-137160 ±300	-121040 ±500	88.72	13
CaO	Lime	56.08	16.76 ±.01	9.5 ±.2	1	-151790 ±300	-144350 ±350	105.81	14
$Ca(OH)_2$	Portlandite	74.096	33.06 ±.04	19.93 ±.10	1	-235610 ±450	-214665 ±500	157.34	15, 16
CdO		128.41	15.59 ±.01	13.1 ±.3	1	-61200 ±200	-53037 ±250	38.87	17
CO	Ideal Gas	28.011	24466.1 ±1.0	47.22 ±.02	18, 8	-26416 ±60	-32844 ±80	24.07	8
CO_2	Ideal Gas	44.011	24466.1 ±1.0	51.07 ±.02	18, 8	-94054 ±30	-94265 ±50	69.095	8
CeO_2	Cerianite	172.13	23.86 ±.02	14.89 ±.03	19	-260180 ±350	-245046 ±450	179.61	20

OXIDES AND HYDROXIDES (Cont.)

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
CoO		74.94	11.64 ±.01	12.66 ±.08	1	-57100 ±300	-51428 ±350	37.70	21
Cr_2O_3	Eskolaite	152.02	28.98 ±.05	19.4 ±.3	1	-272700 ±400	-253200 ±500	185.59	17
CuO	Tenorite	79.54	12.22 ±.02	10.19 ±.05	1	-37140 ±300	-30494 ±350	22.35	22
Cu_2O	Cuprite	143.08	23.44 ±.02	22.4 ±.2	1	-40400 ±1500	-35018 ±1600	25.67	12
$Fe_{.947}O$	Wustite	68.89	12.04 ±.04	13.74 ±.10	1	-63800 ±400	-58760 ±500	43.07	12
Fe_2O_3	Hematite	159.70	30.28 ±.02	20.89 ±.05	23	-196750 ±1100	-177159 ±1400	129.85	24
Fe_3O_4	Magnetite	231.55	44.53 ±.02	36.03 ±.10	25	-267400 ±500	-243113 ±700	178.20	26
H_2O	Water	18.016	18.069 ±.003	16.715 ±.03	27	-68317 ±10	-56688 ±15	41.55	12
H_2O	Ideal Gas	18.016	24466.1 ±1.0	45.106 ±.01	18	-57798 ±10	-54634 ±15	40.06	12
HfO_2	Hafnia	210.50	20.82 ±.01	14.18 ±.10	1	-266050 ±300	-252413 ±350	185.01	12
HgO	Montroydite (red)	216.61	19.32 ±.02	16.80 ±.08	1	-21711 ±90	-13990 ±50	10.254	12
MgO	Periclase	40.32	11.25 ±.01	6.44 ±.04	28	-143800 ±100	-136085 ±150	99.75	12
$Mg(OH)_2$	Brucite	58.336	24.64 ±.03	15.09 ±.05	1	-221200 ±500	-199450 ±550	146.19	29

OXIDES AND HYDROXIDES (Cont.)

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
MnO	Manganosite	70.94	13.22 ±.01	14.27 ±.10	1	-92050 ±110	-86708 ±150	63.55	12
MnO_2	Pyrolusite	86.94	17.16 ±.08	12.68 ±.10	1	-124450 ±200	-111337 ±250	81.608	12
Mn_2O_3	Bixbyite	157.88	31.38 ±.03	26.40 ±.50	1	-229200 ±2000	-210600 ±2200	154.36	12
Mn_3O_4	Hausmannite	228.82	46.96 ±.08	35.5 ±1.0	1	-331400 ±400	-305950 ±800	224.25	12
MoO_3	Molybdite	143.95	30.72 ±.02	18.58 ±.10	1	-178100 ±100	-154445 ±150	113.21	10
NiO	Bunsenite	74.71	10.97 ±.01	9.08 ±.04	1	-57300 ±100	-50572 ±150	37.07	21
PbO	Litharge (red)	223.21	23.91 ±.02	15.6 ±.2	1	-52523 ±300	-45250 ±150	33.17	12
PbO	Massicot (yellow)	223.21	23.15 ±.02	16.1 ±.2	1	-52174 ±300	-45050 ±150	33.02	12
SO_2	Ideal Gas	64.066	24466.1 ±1.0	59.29 ±.10	30	-70947 ±50	-71740 ±60	52.58	30
SO_3	Ideal Gas	80.066	24466.1 ±1.0	61.20 ±.50	1	-94470 ±70	-88526 ±100	64.89	30
Sb_2O_3	Valentinite	291.52	50.01 ±.06	29.4 ±.6	1	-168766 ±1400	-149100 ±1000	109.29	12
SiO_2	α-Quartz	60.09	22.690 ±.005	9.88 ±.02	31	-217650 ±400	-204643 ±500	150.00	32, 92
SiO_2	α-Cristobalite	60.09	25.74 ±.02	10.38 ±.02	31	-216930 ±800	-204072 ±900	149.58	33

OXIDES AND HYDROXIDES (Cont.)

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
SiO_2	α-Tridymite	60.09	26.53 ±.20	10.50 ±.10	86, 1	-216900 ±900	-204077 ±1000	149.59	33
SiO_2	Coesite	60.09	20.64 ±.05	9.30 ±.50	34				
SnO_2	Cassiterite	150.70	21.55 ±.02	12.5 ±.3	1	-138820 ±150	-124270 ±200	91.09	12
TeO_2	Tellurite	159.61	27.75 ±.02	16.8 ±1.0	1	-77745 ±800	-64600 ±700	47.35	12
ThO_2	Thorianite	264.05	26.38 ±.01	15.59 ±.05	1	-293200 ±400	-279431 ±450	204.82	12
TiO_2	Rutile	79.90	18.80 ±.02	12.04 ±.04	1	-225760 ±100	-212552 ±150	155.80	35
TiO_2	Anatase	79.90	20.49 ±.03	11.93 ±.07	1				
UO_2	Uraninite	270.07	24.62 ±.01	18.63 ±.10	1	-259200 ±600	-246556 ±700	180.72	12
ZnO	Zincite	81.38	14.34 ±.01	10.43 ±.10	1	-83250 ±200	-76100 ±200	55.78	12
ZrO_2	Baddeleyite	123.22	21.15 ±.06	12.12 ±.08	1	-261500 ±200	-247732 ±300	181.58	12
Na_2O	Sodium Oxide	61.982		17.99 ±.20	91				

SPINELS, ALUMINATES AND TITANATES

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
$MgAl_2O_4$	Spinel	142.28	39.72 ±.03	19.26 ±.10	1				
$FeAl_2O_4$	Hercynite	173.81	40.82 ±.06	25.4 ±.2	1				
$MgFe_2O_4$	Magnesioferrite	200.02		29.6 ±.6	1	-341171 ±700	-314573 ±1000	230.58	36
$NiFe_2O_4$	Trevorite	234.41	43.66 ±.08	31.5 ±.2	1				
$MgCr_2O_4$	Picrochromite	192.34	43.57 ±.06	25.3 ±.2	1				
$FeCr_2O_4$	Chromite	223.87	44.01 ±.10	34.90 ±.40	1				
$CaTiO_3$	Perovskite	135.98	33.72 ±.08	22.4 ±.1	1	-396900 ±600	-376507 ±700	275.97	37
$FeTiO_3$	Ilmenite	151.75	31.71 ±.05	25.3 ±.3	1	-295560 ±600	-277063 ±700	203.08	37
Fe_2TiO_4	Titanomagnetite	223.60		40.36 ±.60	1				
$MgTiO_3$	Geikielite	120.22	30.86 ±.03	17.82 ±.10	1	-375900 ±400	-354780 ±500	260.05	37

PHOSPHATES, MOLYBDATES AND TUNGSTATES

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
$AlPO_4$	Berlinite	121.955	46.59 ±.05	21.70 ±.05	38				
$Ca_5(PO_4)_3OH$	Hydroxylapatite	502.333	159.66 ±.40	93.30 ±.40	1				
$Ca_5(PO_4)_3F$	Fluorapatite	504.325	157.60 ±.50	92.70 ±.40	1				
$Fe(PO_4)\cdot 2H_2O$	Strengite	186.857		40.93 ±.30	82	-451500 ±1000	-397693 ±1300	291.50	82

CARBONATES AND NITRATES

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
$CaCO_3$	Calcite	100.091	36.94 ±.02	22.2 ±.2	1	-288086 ±250	-269820 ±200	197.77	39, 4
$CaMg(CO_3)_2$	Dolomite	184.422	64.35 ±.04	37.09 ±.07	40	-557567 ±800	-518676 ±900	380.18	40
$CdCO_3$	Otavite	172.421	34.30 ±.02	23.3 ±.6	1	-179040 ±600	-149225 ±1000	109.40	4
$FeCO_3$	Siderite	115.861	29.38 ±.02	23.9 ±.6	41	-178200 ±1200	-161060 ±800	118.05	4,41
$MgCO_3$	Magnesite	84.331	28.02 ±.01	15.7 ±.2	1	-266052 ±400	-246077 ±450	180.37	40
$Mg_3Ca(CO_3)_4$	Huntite	353.084	122.90 ±.30				-1007700 ±1000	738.63	39
$MnCO_3$	Rhodochrosite	114.951	31.08 ±.01	23.90 ±.50	41	-212392 ±800	-194190 ±1000	142.34	42
$ZnCO_3$	Smithsonite	125.391	28.28 ±.01	19.70 ±.30	1	-194200 ±700	-174780 ±1000	128.11	4
$BaCO_3$	Witherite	197.371	45.81 ±.04	26.8 ±.5	1	-291300 ±1100	-272193 ±1500	199.51	4
$CaCO_3$	Aragonite	100.091	34.16 ±.02	21.2 ±.3	1	-288134 ±250	-269570 ±200	197.59	4,39
$PbCO_3$	Cerussite	267.221	40.60 ±.03	31.3 ±.8	1	-167300 ±700	-149690 ±1000	109.72	4
$SrCO_3$	Strontianite	147.641	39.01 ±.03	23.2 ±.4	1	-290728 ±500	-272000 ±200	199.37	39, 43
$Cu_2(OH)_2CO_3$	Malachite	221.107	54.86 ±.05				-216440 ±500	158.65	44

CARBONATES AND NITRATES (Cont.)

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
$Cu_3(OH)_2(CO_3)_2$	Azurite	344.358	91.02 ±.07				-343730 ±500	251.95	44
KNO_3	Niter	101.108	48.04 ±.05	31.81 ±.15	1	-117760 ±300	-93914 ±500	68.84	4
$NaNO_3$	Soda Niter	84.999	37.60 ±.02	27.85 ±.10	1	-111540 ±300	-87461 ±500	64.11	4

SULFATES AND BORATES

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
$BaSO_4$	Barite	233.426	52.11 ±.05	31.6 ±.2	1	-351996 ±2300	-325300 ±2000	238.44	45
$CaSO_4$	Anhydrite	136.146	45.94 ±.05	25.5 ±.4	1	-343335 ±1000	-316475 ±1000	231.97	45, 46
H_2SO_4	Sulfuric Acid	98.082	53.57 ±.07	37.50 ±.05	27	-194670 ±100	-165049 ±150	120.98	47, 27
$PbSO_4$	Anglesite	303.276	47.96 ±.05	35.51 ±.07	48	-220028 ±300	-194500 ±200	142.57	45
$SrSO_4$	Celestite	183.696	46.25 ±.05	28.2 ±1.0	1	-346646 ±1800	-319830 ±1500	234.43	45
$ZnSO_4$	Zinkosite	161.446	41.58 ±.05	27.0 ±1.0	1	-235488 ±1500	-209074 ±900	153.25	45
K_2SO_4	Arcanite	174.266	65.51 ±.07	42.0 ±.4	1	-343704 ±800	-315565 ±500	231.30	45
Na_2SO_4	Thenardite	142.048	53.34 ±.06	35.73 ±.07	1	-331839 ±550	-303715 ±500	222.62	45
$CaSO_4 \cdot 2H_2O$	Gypsum	172.178	74.31 ±.16	46.36 ±.3	4	-484000 ±1100	-430137 ±1000	315.28	45
$MgSO_4 \cdot 7H_2O$	Epsomite	246.498	146.85 ±.50			-808700 ±2000			4
$Na_2SO_4 \cdot 10H_2O$	Mirabilite	322.208	219.83 ±.40	141.46 ±.15	49	-871850 ±700	-709135 ±700	519.78	45
$CuSO_4 \cdot 5H_2O$	Chalcanthite	249.686	109.08 ±.20	73.0 ±1.0	4	-544450 ±1000	-449300 ±1200	329.33	4
$Cu_4SO_4(OH)_6$	Brochantite	452.274	113.60 ±1.15	70.2 ±4.0	22	-527135 ±1200	-435311 ±600	319.08	22

SULFATES AND BORATES (Cont.)

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
$Na_2B_4O_7\text{-}10H_2O$	Borax	381.422	222.68 ±.40			-1497200 ±2000			4

SILICATES

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
Al_2SiO_5	Andalusite	162.05	51.54 ±.01	22.28 ±.10	1				
Al_2SiO_5	Kyanite	162.05	44.11 ±.02	20.02 ±.08	1				
Al_2SiO_5	Sillimanite	162.05	49.91 ±.02	22.97 ±.10	1				
$CaSiO_3$	Wollastonite	116.17	39.94 ±.08	19.60 ±.20	1	-21250 ±700	-21316 ±800	15.624	50, 85
$CaSiO_3$	Pseudowollastonite	116.17	40.08 ±.08	20.90 ±.20	1				
$CaMg(SiO_3)_2$	Diopside	216.58	66.10 ±.10	34.20 ±.20	1	-36500 ±1500	-36053 ±1700	26.426	51, 52
$MgSiO_3$	Clinoenstatite	100.41	31.47 ±.07	16.22 ±.10	1	-8690 ±150	-8660 ±200	5.028	50
$MnSiO_3$	Rhodonite	131.03	35.32 ±.30	24.50 ±.50	41	-5920 ±170	-6024 ±400	4.415	53
$NaAlSi_2O_6$	Jadeite	202.151	60.98 ±.40	31.90 ±.30	1	-36500 ±1000	-35620 ±1400	26.110	51 54
$Ca_2Mg_5Si_8O_{22}(OH)_2$	Tremolite	812.496	272.95 ±.90	131.19 ±.30	40	-120840 ±2500	-116138 ±3000	85.127	55
$CaTiSiO_5$	Sphene	196.07	55.70 ±.30	30.88 ±.20	1	-26850 ±250	-26689 ±350	19.563	56
γ-Ca_2SiO_4	Lime Olivine	172.25	58.63 ±.35	28.80 ±.20	1	-32743 ±600	-32719 ±700	23.982	57
Fe_2SiO_4	Fayalite	203.79	46.39 ±.08	34.70 ±.40	1	-8282 ±400	-7280 ±500	5.336	53 see note a

SILICATES (Cont.)

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
$CaAl_2Si_2O_8$	Anorthite	278.22	100.73 ±.15	48.45 ±.30	1	-21810 ± 700	-23900 ± 900	17.518	54 62
$NaAlSi_3O_8$	Albite	262.241	100.21 ±.19	50.20 ±.40	1	-35900 ±1500	-37530 ±1800	27.509	54
$KAlSi_3O_8$	Orthoclase	278.35		52.47 ±.60	1	-51030 ±1000			54
$KAlSiO_4$	Kaliophillite	158.17	59.90 ±.08	31.85 ±.30	1				
$KAlSi_2O_6$	Leucite	218.26		44.05 ±.40	1	-46200 ±1500			54
$NaAlSiO_4$	Nephelite	142.061	54.17 ±.15	29.72 ±.30	1	-30900 ±1000	-32320 ±1300	23.690	54
$NaAlSi_2O_6 \cdot H_2O$	Analcite	220.167	97.50 ±.10	56.03 ±.60	1	-32750 ±700	-34080 ±900	24.98	94
$NaAlSi_2O_6$	Dehydrated Analcite	202.151		41.93 ±.40	84	-25580 ±700	-27690 ±1000	20.296	54
$CaAl_2Si_2O_8$	Hexagonal Anorthite	278.22		45.84 ±.30	84	-16920 ±600	-18230 ±800	13.36	94
$CaAl_2Si_2O_7(OH)_2 \cdot H_2O$	Lawsonite	314.252	101.33 ±.15	56.79 ±.50	84	-37190 ±600	-31800 ±800	23.31	94
$Ca_2Al_4Si_8O_{24} \cdot 7H_2O$	Leonhardite	922.91		220.40 ±1.60	84	-73740 ±1500	-68075 ±2000	49.90	94
$Ca_2MgSi_2O_7$	Akermanite	272.68	92.82 ±.15			-43830 ±700			52

note a. For the reaction: $2Fe_{.947}O + .106\ Fe + SiO_2 = Fe_2SiO_4$

note b. For the reaction: $KF + 1/2\ MgF_2 + 5/2\ MgO + 1/2\ Al_2O_3 + 3SiO_2 = KMg_3AlSi_3O_{10}F_2$

SILICATES (Cont.)

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
Mg_2SiO_4	Forsterite	140.73	43.67 ±.08	22.75 ±.20	1	-15120 ±250	-15117 ±350	11.081	50
Mn_2SiO_4	Tephroite	201.97	48.62 ±.10	39.00 ±1.00	1	-11770 ±600	-11943 ±1000	8.754	58
$CaMgSiO_4$	Monticellite	156.49	51.37 ±.15			-27560 ±600			52
β-Ca_2SiO_4	Larnite	172.25	51.60 ±.40	30.50 ±.20	1	-30190 ±250	-30673 ±350	22.483	57
Be_2SiO_4	Phenacite	110.116	37.20 ±.06	15.37 ±.08	1				
Zn_2SiO_4	Willemite	222.85	52.42 ±.13	31.40 ±.20	1	-6990 ±140	-7187 ±±400	52.680	57
$ZrSiO_4$	Zircon	183.31	39.27 ±.15	20.20 ±.20	1				
$Mg_3Si_4O_{10}(OH)_2$	Talc	379.336	134.30 ±.80	62.34 ±.15	40	-43600 ±2000	-39658 ±2300	29.069	40
$KMg_3AlSi_3O_{10}F_2$	Fluorphlogopite	421.31	146.38 ±.50	75.90 ±.50	1	-20880 ±2000			59 see note b
$KMg_3AlSi_3O_{10}(OH)_2$	Phlogopite	417.326	149.66 ±1.00	75.20 ±1.00	60				
$Al_2Si_2O_5(OH)_4$	Kaolinite	258.172		48.53 ±.30	61	-7140 ±500	-1982 ±700	1.453	11
$Al_2Si_2O_5(OH)_4$	Dickite	258.172	99.31 ±.30	47.10 ±.30	61	-6840 ±500	-1390 ±700	1.019	11
$Al_2Si_2O_5(OH)_4$	Halloysite	258.172		48.63 ±.30	61	-2670 ±500	+2324 ±700	-1.703	11

SULFIDES, TELLURIDES AND SELENIDES

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
Ag_2S	Acanthite (Argentite)	247.826	34.21 ±.05	34.14 ±.10	63	-7737 ±300	-9562 ±200	7.009	64, 65, 66
CaS	Oldhamite	72.146	27.81 ±.02	13.54 ±.30	1	-114390 ±600	-113070 ±500	82.878	67
CdS	Greenockite	144.476	29.94 ±.02	16.80 ±.40	1				
CuS	Covellite	95.606	20.43 ±.04	15.93 ±.40	1				
Cu_2S	Chalcocite	127.672	27.47 ±.06	28.86 ±.50	1	-19148 ±300	-20728 ±300	15.193	68, 69, 70
FeS	Troilite (Pyrrhotite)	87.916	18.17 ±.05	14.42 ±.04	71	-24220 ±250	-24311 ±300	17.820	72, 73, 74
FeS_2	Pyrite	119.982	23.94 ±.02	12.65 ±.03	63	-41000 ±400	-38293 ±450	28.068	75
$FeSe_2$	Ferroselite	134.81	29.92 ±.08	20.76 ±.06	63				
H_2S	Ideal Gas	34.082	24466.1 ±1.0	49.13 ±.10	1	-4815 ±100	-7890 ±100	5.783	29
HgS	Metacinnabar	232.676	30.17 ±.04	23.00 ±1.00	1	-11058 ±500	-10220 ±200	7.491	76
α-MnS	Alabandite	87.006	21.46 ±.01	18.69 ±.40	1	-49000 ±400	-50020 ±400	35.169	77
MoS_2	Molybdenite	160.082	32.03 ±.07	14.96 ±.05	63	-60500 ±1500	-58380 ±1500	42.792	88
NiS	Millerite	90.776	50.68 ±.05	15.80 ±1.00	63	-20290 ±1000	-20600 ±1000	15.099	83

SULFIDES, TELLURIDES AND SELENIDES

Formula	Name	Formula weight grams	Molar volume cm^3	Entropy $S^\circ_{298.15}$ cal/gfw deg	Ref.	$\Delta H^\circ_{f,298.15}$ cal/gfw	$\Delta F^\circ_{f,298.15}$ cal/gfw	Log K_f	Ref.
PbS	Galena	239.276	31.49 ±.01	21.84 ±.30	1	-23360 ±250	-22980 ±200	16.844	64, 78
PbSe	Clausthalite	286.17	34.61 ±.01	24.48 ±.50	1				
PbTe	Altaite	334.82	40.60 ±.01	26.26 ±.50	1	-16921 ±500	-16590 ±300	12.160	79
PtS	Cooperite	227.156	22.15 ±.02	13.16 ±.03	63	-19700 ±800	-18370 ±900	13.465	63
SnS	Herzenbergite	150.766	29.01 ±.02	18.36 ±.20	1	-25400 ±300	-23950 ±350	17.555	80
WS_2	Tungstenite	247.992	32.07 ±.05	22.70 ±2.0	63				
ZnS	Sphalerite	97.446	23.83 ±.01	13.77 ±.20	1	-49200 ±1000	-48067 ±1100	35.32	81
S_2	**Ideal Gas**	**64.132**	24466.1 ±1.0	**54.51 ±.10**	**8**	**30840 ±200**	**19138 ±200**	**-14.028**	**8**
S_8	**Ideal Gas**	**256.528**	24466.1 ±1.0	**103.30 ±.40**	**8**	**24510 ±50**	**11919 ±150**	**-8.736**	**8**

H_2O, IDEAL GAS

Reference states:
for elements from Stull and Sinke 93 ; for H_2O ideal gas 298.15° to 1800°K.

Gram formula weight	18.016 gms
Gfw volume	24466 cm^3
Melting point	°K
$\Delta H°_{melting}$	cal
Boiling point	°K
$\Delta H°_{vaporization}$	10518 cal
$H°_{298.15} - H°_0$	cal

Transitions in reference states:

T Temperature °K	$H°_T - H°_{298.15}$ Heat content cal/gfw	$S°_T$ Entropy cal/deg gfw	$-\frac{(F°_T - H°_{298.15})}{T}$ Free energy function cal/deg gfw	Formation from (reference state)- Elements: Heat $\Delta H°_f$ cal/gfw	Elements: Free energy $\Delta F°_f$ cal/gfw	Oxides: Heat $\Delta H°_f$ cal/gfw	Oxides: Free energy $\Delta F°_f$ cal/gfw
298.15	[a] 0	45.106 ±.03	45.106	-57798 ±30	-54636 ±30		
400	825	47.484	45.422	-58042	-53519		
500	1654	49.334	46.026	-58277	-52361		
600	2509	50.891	46.701	-58500	-51156		
700	3390	52.249	47.406	-58710	-49915		
800	4300	53.464	48.089	-58905	-48646		
900	5240	54.570	48.749	-59084	-47352		
1000	6209	55.592	49.382	-59246	-46040		
1100	7210	56.545	49.991	-59391	-44712		
1200	8240	57.441	50.575	-59519	-43317		
1300	9298	58.288	51.136	-59634	-42022		
1400	10384	59.092	51.675	-59734	-40663		
1500	11495	59.859	52.196	-59824	-39297		
1600	12630	60.591	52.698	-59906	-37927		
1700	13787	61.293	53.183	-59977	-36549		
1800	14964	61.965	53.652	-60041	-35170		

[a] Table modified from Hilsenrath, U. S. Nat. Bur. Stds. Cir. 564, 1955.

CO_2 IDEAL GAS

Reference states:
for elements from Stull and Sinke 93 ; for CO_2, ideal gas 298° to 1800°K.

Gram formula weight	44.011 gms
Gfw volume	24466 cm^3
Melting point	°K
$\Delta H°_{melting}$	cal
Boiling point	°K
$\Delta H°_{vaporization}$	cal
$H°_{298.15} - H°_0$	cal

Transitions in reference states:

T Temperature °K	$H°_T - H°_{298.15}$ Heat content cal/gfw	$S°_T$ Entropy cal/deg gfw	$-\frac{(F°_T - H°_{298.15})}{T}$ Free energy function cal/deg gfw	Formation from (reference state)- Elements: Heat $\Delta H°_f$ cal/gfw	Elements: Free energy $\Delta F°_f$ cal/gfw	Oxides: Heat $\Delta H°_f$ cal/gfw	Oxides: Free energy $\Delta F°_f$ cal/gfw
298.15	[a] 0	51.073 (±.05)	51.073	[b] -94052 (±10)	-94259 (±30)		
400	956.9	53.824	51.432	-94069	-94317		
500	1985.3	56.116	52.145	-94090	-94374		
600	3085.1	58.119	52.997	-94123	-94440		
700	4243.7	59.904	53.842	-94165	-94480		
800	5451.3	61.516	54.702	-94216	-94526		
900	6699.9	62.986	55.541	-94269	-94558		
1000	7982.7	64.337	56.354	-94319	-94586		
1100	9293.9	65.587	57.138	-94367	-94622		
1200	10630	66.748	57.890	-94410	-94616		
1300	11986	67.835	58.615	-94464	-94656		
1400	13360	68.854	59.311	-94516	-94683		
1500	14748	69.812	59.980	-94571	-94682		
1600	16150	70.714	60.620	-94626	-94676		
1700	17563	71.571	61.240	-94681	-94681		
1800	18985	72.383	61.836	-94740	-94675		

[a] Calculated from Circular 564, National Bureau of Standards (1955).

[b] Coughlin, J. P., U. S. Bur. Mines Bull. 542, (1954).

S_2, IDEAL DIATOMIC GAS

Reference states:
for sulfur from JANAF tables 8 ; for S_2 ideal diatomic gas 298.15° to 1800°K.

Gram formula weight	64.132 gms
Gfw volume	24466 cm^3
Melting point	°K
$\Delta H°_{melting}$	cal
Boiling point	°K
$\Delta H°_{vaporization}$	cal
$H°_{298.15} - H°_0$	cal

Transitions in reference states:

$S_{orth} - S_{mon\ I}$	368.54°K
$S_{mon\ I} - S_{mon\ II}$	374.15°K
$S_{mon\ II}$ M.P.	388.36°K
$S_{liq\ I} - S_{liq\ II}$	433.15°K
$S_{liq\ II}$ B.P.	717.75°K

T Temperature °K	$H°_T - H°_{298.15}$ Heat content cal/gfw	$S°_T$ Entropy cal/deg gfw	$-\frac{(F°_T - H°_{298.15})}{T}$ Free energy function cal/deg gfw	Formation from (reference state)- Elements: Heat $\Delta H°_f$ cal/gfw	Elements: Free energy $\Delta F°_f$ cal/gfw	Oxides: Heat $\Delta H°_f$ cal/gfw	Oxides: Free energy $\Delta F°_f$ cal/gfw
298.15	[a] 0	54.510 ±.03	54.510	30840 ±150	19138 ±200		
400	811	56.848	54.819	29433	15233		
500	1639	58.693	55.416	28385	11806		
600	2486	60.238	56.094	27518	8575		
700	3347	61.564	56.783	26779	5525		
800	4217	62.726	57.455	0	0		
900	5093	63.758	58.099	0	0		
1000	5975	64.687	58.712	0	0		
1100	6860	65.531	59.294	0	0		
1200	7749	66.304	59.846	0	0		
1300	8640	67.017	60.371	0	0		
1400	9533	67.679	60.870	0	0		
1500	10428	68.296	61.344	0	0		
1600	11325	68.875	61.797	0	0		
1700	12223	69.420	62.230	0	0		
1800	13123	69.934	62.643	0	0		

[a] Entire table taken from JANAF Interim Thermochem. Tables, Dow Chemical Co., 1960-2.

H_2O
STEAM

PRESSURE BARS.	CHANGE IN FREE ENERGY WITH PRESSURE, $F_{P,T} - F^{\circ}_{T,}$ calories											
	TEMPERATURE °K											
			650	700	750	800	850	900	950	1000	1100	1200	1300
50			4930	5338	5744	6152	6553	6943	7238	7718	8508	9295	10048
100			5719	6217	6698	7184	7658	8130	8596	9065	9990	10923	11851
150			6121	6690	7238	7775	8305	8820	9340	9850	10865	11879	12882
200			6354	6994	7593	8177	8745	9295	9848	10395	11473	12556	13623
250			6474	7202	7851	8472	9074	9655	10238	10816	11942	13070	14182
300			6522	7344	8046	8701	9335	9943	10553	11150	12320	13492	14647
350			6554	7438	8195	8888	9547	10183	10815	11432	12641	13849	15042
400			6590	7502	8312	9039	9724	10387	11033	11668	12916	14153	15380
450			6627	7552	8406	9167	9873	10559	11227	11877	13155	14427	15680
500			6661	7596	8482	9272	10002	10707	11395	12058	13369	14665	15945
550			6693	7638	8545	9365	10118	10841	11543	12226	13565	14880	16185
600			6727	7680	8604	9444	10221	10960	11678	12378	13738	15074	16404
650			6759	7718	8654	9516	10310	11069	11803	12515	13898	15255	16603
700			6792	7755	8700	9580	10394	11166	11915	12637	14043	15425	16790
750			6822	7791	8748	9641	10468	11255	12015	12753	14179	15580	16967
800			6853	7828	8793	9695	10538	11340	12108	12860	14305	15725	17129
850			6885	7863	8834	9747	10603	11417	12200	12959	14428	15864	17283
900			6914	7898	8875	9796	10665	11491	12285	13056	14539	15994	17428
950			6945	7930	8916	9844	10721	11557	12363	13144	14644	16115	17565
1000			6973	7963	8953	9890	10762	11619	12434	13226	14744	16230	17696
1100			7033	8030	9015	9978	10877	11740	12572	13380	14932	16443	17936
1200			7090	8095	9098	10060	10975	11852	12699	13520	15101	16642	18159
1300			7145	8154	9169	10139	11062	11953	12814	13647	15255	16823	18362
1400			7203	8215	9234	10217	11143	12048	12924	13771	15400	16990	18548

Calculated from specific volume for H_2O of:

a. Holser, W. T. and Kennedy, G. C., Am. Jour. Sci. 256, 744, (1958).

b. Holser, W. T. and Kennedy, G. C., Am. Jour. Sci. 257, 71, (1959).

CO_2

PRESSURE BARS.	CHANGE IN FREE ENERGY WITH PRESSURE, $F_{P,T} - F°_{T,}$ calories												
	TEMPERATURE °K												
	400	450	500	550	600	650	700	750	800	900	1000	1100	1200
[a] [b] 100	3503	4002	4495	4977	5456	5937	6408	6878	7391	8269	9190	10137	11058
150	3780	4383	4932	5465	5993	6512	7030	7053	8060	9083	10102	11123	12118
200	3959	4602	5203	5777	6337	6898	7447	8000	8542	9622	10701	11782	12844
250	4085	4763	5395	6002	6595	7195	7762	8340	8902	10038	11163	12290	13407
300	4188	4902	5557	6191	6810	7422	8021	8622	9205	10385	11551	12720	13874
350	4277	5014	5694	6351	6992	7625	8247	8865	9471	10678	11882	13083	14270
400	4357	5115	5818	6494	7155	7803	8445	9080	9700	10938	12176	13397	14616
450	4436	5207	5928	6622	7299	7966	8623	9273	9908	11169	12431	13683	14927
500	4510	5295	6033	6741	7430	8113	8785	9448	10095	11380	12668	13935	15203
600	4643	5453	6214	6949	7670	8372	9065	9751	10422	11755	13080	14388	15698
700	4773	5602	6379	7133	7875	8598	9312	10022	10711	12082	13441	14787	16126
800	4895	5740	6538	7305	8069	8807	9541	10263	10969	12370	13758	15131	16502
900	5010	5871	6683	7472	8242	9002	9747	10482	11202	12629	14049	15451	16846
1000	5128	5998	6827	7623	8406	9180	9942	10685	11420	12871	14317	15743	17147
1100	5236	6122	6958	7764	8563	9348	10117	10878	11624	13098	14567	16019	17430
1200	5346	6241	7086	7909	8714	9507	10288	11063	11822	13316	14795	16268	17703
1300	5451	6355	7213	8046	8861	9666	10455	11233	12001	13516	15018	16503	17961
1400	5557	6470	7340	8171	9001	9813	10614	11404	12184	13710	15225	16723	18200

[a] Hilsenrath and others, U. S. Nat. Bur. Stds. Cir. 564, (1955).

[b] Recalculated from Price, Ind. and Eng. Chem. 47, 1649, (1955).

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