Thermo

Table C.1: Heat Capacities of Gases in the Ideal-Gas State[†]

Constants in equation $C_P^{ig}/R = A + BT + CT^2 + DT^{-2}$ T (kelvins) from 298 to T_{max}

Chemical species		T_{max}	$C_{P_{298}}^{ig}/R$	A	$10^3\,B$	$10^6\,C$	$10^{-5}\,D$
Paraffins:							
Methane	CH_4	1500	4.217	1.702	9.081	−2.164	
Ethane	C_2H_6	1500	6.369	1.131	19.225	−5.561	
Propane	C_3H_8	1500	9.011	1.213	28.785	−8.824	
n-Butane	C_4H_{10}	1500	11.928	1.935	36.915	−11.402	
iso-Butane	C_4H_{10}	1500	11.901	1.677	37.853	−11.945	
n-Pentane	C_5H_{12}	1500	14.731	2.464	45.351	−14.111	
n-Hexane	C_6H_{14}	1500	17.550	3.025	53.722	−16.791	
n-Heptane	C_7H_{16}	1500	20.361	3.570	62.127	−19.486	
n-Octane	C_8H_{18}	1500	23.174	4.108	70.567	−22.208	
1-Alkenes:							
Ethylene	C_2H_4	1500	5.325	1.424	14.394	−4.392	
Propylene	C_3H_6	1500	7.792	1.637	22.706	−6.915	
1-Butene	C_4H_8	1500	10.520	1.967	31.630	−9.873	
1-Pentene	C_5H_{10}	1500	13.437	2.691	39.753	−12.447	
1-Hexene	C_6H_{12}	1500	16.240	3.220	48.189	−15.157	
1-Heptene	C_7H_{14}	1500	19.053	3.768	56.588	−17.847	
1-Octene	C_8H_{16}	1500	21.868	4.324	64.960	−20.521	
Miscellaneous organics:							
Acetaldehyde	C_2H_4O	1000	6.506	1.693	17.978	−6.158	
Acetylene	C_2H_2	1500	5.253	6.132	1.952	.....	−1.299
Benzene	C_6H_6	1500	10.259	−0.206	39.064	−13.301	
1,3-Butadiene	C_4H_6	1500	10.720	2.734	26.786	−8.882	
Cyclohexane	C_6H_{12}	1500	13.121	−3.876	63.249	−20.928	
Ethanol	C_2H_6O	1500	8.948	3.518	20.001	−6.002	
Ethylbenzene	C_8H_{10}	1500	15.993	1.124	55.380	−18.476	
Ethylene oxide	C_2H_4O	1000	5.784	−0.385	23.463	−9.296	
Formaldehyde	CH_2O	1500	4.191	2.264	7.022	−1.877	
Methanol	CH_4O	1500	5.547	2.211	12.216	−3.450	
Styrene	C_8H_8	1500	15.534	2.050	50.192	−16.662	
Toluene	C_7H_8	1500	12.922	0.290	47.052	−15.716	
Miscellaneous inorganics:							
Air		2000	3.509	3.355	0.575	.....	−0.016
Ammonia	NH_3	1800	4.269	3.578	3.020	.....	−0.186
Bromine	Br_2	3000	4.337	4.493	0.056	.....	−0.154
Carbon monoxide	CO	2500	3.507	3.376	0.557	.....	−0.031
Carbon dioxide	CO_2	2000	4.467	5.457	1.045	.....	−1.157
Carbon disulfide	CS_2	1800	5.532	6.311	0.805	.....	−0.906
Chlorine	Cl_2	3000	4.082	4.442	0.089	.....	−0.344
Hydrogen	H_2	3000	3.468	3.249	0.422	.....	0.083
Hydrogen sulfide	H_2S	2300	4.114	3.931	1.490	.....	−0.232
Hydrogen chloride	HCl	2000	3.512	3.156	0.623	.....	0.151
Hydrogen cyanide	HCN	2500	4.326	4.736	1.359	.....	−0.725
Nitrogen	N_2	2000	3.502	3.280	0.593	.....	0.040
Nitrous oxide	N_2O	2000	4.646	5.328	1.214	.....	−0.928
Nitric oxide	NO	2000	3.590	3.387	0.629	.....	0.014
Nitrogen dioxide	NO_2	2000	4.447	4.982	1.195	.....	−0.792
Dinitrogen tetroxide	N_2O_4	2000	9.198	11.660	2.257	.....	−2.787
Oxygen	O_2	2000	3.535	3.639	0.506	.....	−0.227
Sulfur dioxide	SO_2	2000	4.796	5.699	0.801	.....	−1.015
Sulfur trioxide	SO_3	2000	6.094	8.060	1.056	.....	−2.028
Water	H_2O	2000	4.038	3.470	1.450	.....	0.121

[†]Selected from H. M. Spencer, *Ind. Eng. Chem.*, vol. 40, pp. 2152–2154, 1948; K. K. Kelley, *U.S. Bur. Mines Bull. 584*, 1960; L. B. Pankratz, *U.S. Bur. Mines Bull. 672*, 1982.

Table C.2: Heat Capacities of Solids†

Constants for the equation $C_P/R = A + BT + DT^{-2}$
T (kelvins) from 298 K to T_{max}

Chemical species	T_{max}	$C_{P_{298}}/R$	A	$10^3\,B$	$10^{-5}\,D$
CaO	2000	5.058	6.104	0.443	−1.047
$CaCO_3$	1200	9.848	12.572	2.637	−3.120
$Ca(OH)_2$	700	11.217	9.597	5.435	
CaC_2	720	7.508	8.254	1.429	−1.042
$CaCl_2$	1055	8.762	8.646	1.530	−0.302
C (graphite)	2000	1.026	1.771	0.771	−0.867
Cu	1357	2.959	2.677	0.815	0.035
CuO	1400	5.087	5.780	0.973	−0.874
Fe (α)	1043	3.005	−0.111	6.111	1.150
Fe_2O_3	960	12.480	11.812	9.697	−1.976
Fe_3O_4	850	18.138	9.594	27.112	0.409
FeS	411	6.573	2.612	13.286	
I_2	386.8	6.929	6.481	1.502	
LiCl	800	5.778	5.257	2.476	−0.193
NH_4Cl	458	10.741	5.939	16.105	
Na	371	3.386	1.988	4.688	
NaCl	1073	6.111	5.526	1.963	
NaOH	566	7.177	0.121	16.316	1.948
$NaHCO_3$	400	10.539	5.128	18.148	
S (rhombic)	368.3	3.748	4.114	−1.728	−0.783
SiO_2 (quartz)	847	5.345	4.871	5.365	−1.001

†Selected from K. K. Kelley, *U.S. Bur. Mines Bull. 584*, 1960; L. B. Pankratz, *U.S. Bur. Mines Bull. 672*, 1982.

Table C.3: Heat Capacities of Liquids†

Constants for the equation $C_P/R = A + BT + CT^2$
T from 273.15 to 373.15 K

Chemical species	$C_{P_{298}}/R$	A	$10^3\,B$	$10^6\,C$
Ammonia	9.718	22.626	−100.75	192.71
Aniline	23.070	15.819	29.03	−15.80
Benzene	16.157	−0.747	67.96	−37.78
1,3-Butadiene	14.779	22.711	−87.96	205.79
Carbon tetrachloride	15.751	21.155	−48.28	101.14
Chlorobenzene	18.240	11.278	32.86	−31.90
Chloroform	13.806	19.215	−42.89	83.01
Cyclohexane	18.737	−9.048	141.38	−161.62
Ethanol	13.444	33.866	−172.60	349.17
Ethylene oxide	10.590	21.039	−86.41	172.28
Methanol	9.798	13.431	−51.28	131.13
n-Propanol	16.921	41.653	−210.32	427.20
Sulfur trioxide	30.408	−2.930	137.08	−84.73
Toluene	18.611	15.133	6.79	16.35
Water	9.069	8.712	1.25	−0.18

†Based on correlations presented by J. W. Miller, Jr., G. R. Schorr, and C. L. Yaws, *Chem. Eng.*, vol. 83(23), p. 129, 1976.

Table C.4: Standard Enthalpies and Gibbs Energies of Formation at 298.15 K†

Joules per mole of the substance formed

Chemical species		State (Note 2)	$\Delta H^\circ_{f_{298}}$ (Note 1)	$\Delta G^\circ_{f_{298}}$ (Note 1)
Paraffins:				
Methane	CH_4	(*g*)	−74,520	−50,460
Ethane	C_2H_6	(*g*)	−83,820	−31,855
Propane	C_3H_8	(*g*)	−104,680	−24,290
n-Butane	C_4H_{10}	(*g*)	−125,790	−16,570
n-Pentane	C_5H_{12}	(*g*)	−146,760	−8,650
n-Hexane	C_6H_{14}	(*g*)	−166,920	150
n-Heptane	C_7H_{16}	(*g*)	−187,780	8,260
n-Octane	C_8H_{18}	(*g*)	−208,750	16,260
1-Alkenes:				
Ethylene	C_2H_4	(*g*)	52,510	68,460
Propylene	C_3H_6	(*g*)	19,710	62,205
1-Butene	C_4H_8	(*g*)	−540	70,340
1-Pentene	C_5H_{10}	(*g*)	−21,280	78,410
1-Hexene	C_6H_{12}	(*g*)	−41,950	86,830
1-Heptene	C_7H_{14}	(*g*)	−62,760	
Miscellaneous organics:				
Acetaldehyde	C_2H_4O	(*g*)	−166,190	−128,860
Acetic acid	$C_2H_4O_2$	(*l*)	−484,500	−389,900
Acetylene	C_2H_2	(*g*)	227,480	209,970
Benzene	C_6H_6	(*g*)	82,930	129,665
Benzene	C_6H_6	(*l*)	49,080	124,520
1,3-Butadiene	C_4H_6	(*g*)	109,240	149,795
Cyclohexane	C_6H_{12}	(*g*)	−123,140	31,920
Cyclohexane	C_6H_{12}	(*l*)	−156,230	26,850
1,2-Ethanediol	$C_2H_6O_2$	(*l*)	−454,800	−323,080
Ethanol	C_2H_6O	(*g*)	−235,100	−168,490
Ethanol	C_2H_6O	(*l*)	−277,690	−174,780
Ethylbenzene	C_8H_{10}	(*g*)	29,920	130,890
Ethylene oxide	C_2H_4O	(*g*)	−52,630	−13,010
Formaldehyde	CH_2O	(*g*)	−108,570	−102,530
Methanol	CH_4O	(*g*)	−200,660	−161,960
Methanol	CH_4O	(*l*)	−238,660	−166,270
Methylcyclohexane	C_7H_{14}	(*g*)	−154,770	27,480
Methylcyclohexane	C_7H_{14}	(*l*)	−190,160	20,560
Styrene	C_8H_8	(*g*)	147,360	213,900
Toluene	C_7H_8	(*g*)	50,170	122,050
Toluene	C_7H_8	(*l*)	12,180	113,630

Table C.4 (Continued)

Chemical species		State (Note 2)	ΔH°_{f298} (Note 1)	ΔG°_{f298} (Note 1)
Miscellaneous inorganics:				
Ammonia	NH_3	(*g*)	−46,110	−16,450
Ammonia	NH_3	(*aq*)		−26,500
Calcium carbide	CaC_2	(*s*)	−59,800	−64,900
Calcium carbonate	$CaCO_3$	(*s*)	−1,206,920	−1,128,790
Calcium chloride	$CaCl_2$	(*s*)	−795,800	−748,100
Calcium chloride	$CaCl_2$	(*aq*)		−8,101,900
Calcium chloride	$CaCl_2 \cdot 6H_2O$	(*s*)	−2,607,900	
Calcium hydroxide	$Ca(OH)_2$	(*s*)	−986,090	−898,490
Calcium hydroxide	$Ca(OH)_2$	(*aq*)		−868,070
Calcium oxide	CaO	(*s*)	−635,090	−604,030
Carbon dioxide	CO_2	(*g*)	−393,509	−394,359
Carbon monoxide	CO	(*g*)	−110,525	−137,169
Hydrochloric acid	HCl	(*g*)	−92,307	−95,299
Hydrogen cyanide	HCN	(*g*)	135,100	124,700
Hydrogen sulfide	H_2S	(*g*)	−20,630	−33,560
Iron oxide	FeO	(*s*)	−272,000	
Iron oxide (hematite)	Fe_2O_3	(*s*)	−824,200	−742,200
Iron oxide (magnetite)	Fe_3O_4	(*s*)	−1,118,400	−1,015,400
Iron sulfide (pyrite)	FeS_2	(*s*)	−178,200	−166,900
Lithium chloride	LiCl	(*s*)	−408,610	
Lithium chloride	$LiCl \cdot H_2O$	(*s*)	−712,580	
Lithium chloride	$LiCl \cdot 2H_2O$	(*s*)	−1,012,650	
Lithium chloride	$LiCl \cdot 3H_2O$	(*s*)	−1,311,300	
Nitric acid	HNO_3	(*l*)	−174,100	−80,710
Nitric acid	HNO_3	(*aq*)		−111,250
Nitrogen oxides	NO	(*g*)	90,250	86,550
	NO_2	(*g*)	33,180	51,310
	N_2O	(*g*)	82,050	104,200
	N_2O_4	(*g*)	9,160	97,540
Sodium carbonate	Na_2CO_3	(*s*)	−1,130,680	−1,044,440
Sodium carbonate	$Na_2CO_3 \cdot 10H_2O$	(*s*)	−4,081,320	
Sodium chloride	NaCl	(*s*)	−411,153	−384,138
Sodium chloride	NaCl	(*aq*)		−393,133
Sodium hydroxide	NaOH	(*s*)	−425,609	−379,494
Sodium hydroxide	NaOH	(*aq*)		−419,150
Sulfur dioxide	SO_2	(*g*)	−296,830	−300,194
Sulfur trioxide	SO_3	(*g*)	−395,720	−371,060
Sulfur trioxide	SO_3	(*l*)	−441,040	
Sulfuric acid	H_2SO_4	(*l*)	−813,989	−690,003
Sulfuric acid	H_2SO_4	(*aq*)		−744,530
Water	H_2O	(*g*)	−241,818	−228,572
Water	H_2O	(*l*)	−285,830	−237,129

†From *TRC Thermodynamic Tables—Hydrocarbons*, Thermodynamics Research Center, Texas A & M Univ. System, College Station, TX; "The NBS Tables of Chemical Thermodynamic Properties," *J. Phys. and Chem. Reference Data*, vol. 11, supp. 2, 1982.

Notes

1. The standard property changes of formation ΔH°_{f298} and ΔG°_{f298} are the changes occurring when 1 mol of the listed compound is formed from its elements with each substance in its standard state at 298.15 K (25°C).
2. Standard states: (*a*) Gases (*g*): pure ideal gas at 1 bar and 25°C. (*b*) Liquids (*l*) and solids (*s*): pure substance at 1 bar and 25°C. (*c*) Solutes in aqueous solution (*aq*): Hypothetical ideal 1-molal solution of solute in water at 1 bar and 25°C.