Appendix C

Heat Capacities and Property Changes of Formation

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

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

Chemical species		T_{max}	$C_{P_{298}}^{ig}/R$	A	$10^3\,B$	$10^6\,C$	$10^{-5}\,D$
Alkanes:							
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 $C_p/R = A + BT + DT^{-2}$ for T (K) from 298 K to T_{max}

Chemical species	T_{max}	$C^{ig}_{P_{298}}/R$	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 $C_P/R = A + BT + CT^2$ for T from 273.15 to 373.15 K

Chemical species	$C^{ig}_{P_{298}}/R$	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)	ΔH°_{f298} (Note 1)	ΔG°_{f298} (Note 1)
Alkanes:				
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)	$\Delta H^{\circ}_{f_{298}}$ (Note 1)	$\Delta G^{\circ}_{f_{298}}$ (Note 1)
Miscellaneous inorganics:				
Ammonia	NH_3	(*g*)	−46,110	−16,400
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.

Table C.5: Standard Enthalpies and Gibbs Energies of Formation at 298.15 K for Substances in Dilute Aqueous Solution at Zero Ionic Strength†

Joules per mole of the substance formed

Chemical species		ΔH°_{f298}	ΔG°_{f298}
Acetaldehyde	C_2H_4O	−212.2	−139.0
Acetate	$C_2H_2O_2^-$	−486.0	−369.3
Acetic acid	$C_2H_3O_2$	−485.8	−396.5
Acetone	C_3H_6O	−221.7	−159.7
Adenosine	$C_{10}H_{13}N_5O_4$	−621.3	−194.5
Adenosine cation	$C_{10}H_{14}N_5O_4^+$	−637.7	−214.3
Adenosine 5′ diphosphate (ADP)	$C_{10}H_{12}N_5O_{10}P_2^{3-}$	−2626.5	−1906.1
	$C_{10}H_{13}N_5O_{10}P_2^{2-}$	−2620.9	−1947.1
	$C_{10}H_{14}N_5O_{10}P_2^-$	−2638.5	−1972.0
Adenosine 5′ monophosphate (AMP)	$C_{10}H_{12}N_5O_{10}P^{2-}$	−1635.4	−1040.5
	$C_{10}H_{13}N_5O_{10}P^-$	−1630.0	−1078.9
	$C_{10}H_{14}N_5O_7P$	−1648.1	−1101.6
Adenosine 5′ triphosphate (ATP)	$C_{10}H_{12}N_5O_{13}P_3^{4-}$	−3619.2	−2768.1
	$C_{10}H_{13}N_5O_{13}P_3^{3-}$	−3612.9	−2811.5
	$C_{10}H_{14}N_5O_{13}P_3^{2-}$	−3627.9	−2838.2
Alanine	$C_3H_7NO_2$	−554.8	−371.0
Ammonia	NH_3	−80.3	−26.5
Ammonium	NH_4^+	−132.5	−79.3
D-arabinose	$C_5H_{10}O_5$	−1043.8	−742.2
L-asparagine	$C_4H_8N_2O_3$	−766.1	−525.9
L-aspartate	$C_4H_7NO_4$	−943.4	−695.9
Citrate	$C_6H_5O_7^{3-}$	−1515.1	−1162.7
	$C_6H_6O_7^{2-}$	−1518.5	−1199.2
	$C_6H_7O_7^-$	−1520.9	−1226.3
Carbon dioxide	CO_2	−413.8	−386.0
Carbonate	CO_3^{-2}	−677.1	−527.8
Bicarbonate	CHO_3^-	−692.0	−586.8
Carbonic acid	CH_2O_3	−694.9	−606.3

Table C.5 (Continued)

Chemical species		ΔH°_{f298}	ΔG°_{f298}
Carbon monoxide	CO	−121.0	−119.9
Ethanol	C_2H_6O	−288.3	−181.6
Ethyl acetate	$C_4H_8O_2$	−482.0	−337.7
Formate	CHO_2^-	−425.6	−351.0
D-fructose	$C_6H_{12}O_6$	−1259.4	−915.5
D-fructose 6-phosphate	$C_6H_{11}O_9P^{2-}$	−2267.7*	−1760.8
	$C_6H_{12}O_9P^-$	−2265.9*	−1796.6
D-fructose 1,6-biphosphate	$C_6H_{11}O_{12}P_2^{3-}$	−3320.1*	−2639.4
	$C_6H_{12}O_{12}P_2^{2-}$	−3318.3*	−2673.9
Fumarate	$C_4H_2O_4^{2-}$	−777.4	−601.9
	$C_4H_3O_4^-$	−774.5	−628.1
	$C_4H_4O_4$	−774.9	−645.8
D-galactose	$C_6H_{12}O_6$	−1255.2	−908.9
D-glucose	$C_6H_{12}O_6$	−1262.2	−915.9
D-glucose 6-phosphate	$C_6H_{11}O_9P^{2-}$	−2276.4	−1763.9
	$C_6H_{12}O_9P^-$	−2274.6	−1800.6
L-glutamate	$C_5H_8NO_4^-$	−979.9	−697.5
L-glutamine	$C_5H_{10}N_2O_3$	−805.0	−528.0
Glycerol	$C_3H_8O_3$	−676.6	−497.5
Glycine	$C_2H_5NO_2$	−523.0	−379.9
Glycylglycine	$C_4H_8N_2O_3$	−734.3	−520.2
Hydrogen	H_2	−4.2	17.6
Hydrogen peroxide	H_2O_2	−191.2	−134.0
Hydrogen ion (Note 2)	H^+	0.0	0.0
Indole	C_8H_7N	97.5	223.8
Lactate	$C_3H_5O_3^-$	−686.6	−516.7
Lactose	$C_{12}H_{22}O_{11}$	−2233.1	−1567.3
L-leucine	$C_6H_{13}NO_2$	−643.4	−352.3
Maltose	$C_{12}H_{22}O_{11}$	−2238.1	−1574.7
D-mannose	$C_6H_{12}O_6$	−1258.7	−910.0
Methane	CH_4	−89.0	−34.3
Methanol	CH_4O	−245.9	−175.3
Methylammonium	CH_6N^+	−124.9	−39.9
Nitrogen	N_2	−10.5	18.7
Nicotinamide-adenine dinucleotide (ox)	NAD^+ (Note 2)	0.0	0.0
Nicotinamide-adenine dinucleotide (red)	NADH (Note 2)	−31.9	22.7
Nicotinamide-adenine dinucleotide phosphate (ox)	$NADP^+$ (Note 2)	0.0	−835.2

Table C.5 (Continued)

Chemical species		$\Delta H^\circ_{f_{298}}$	$\Delta G^\circ_{f_{298}}$
Nicotinamide-adenine dinucleotide phosphate (red)	NADPH (Note 2)	−29.2	−809.2
Oxygen	O_2	−11.7	16.4
Oxalate	$C_2O_4^{2-}$	−825.1	−673.9
Hydrogen phosphate	HPO_4^{2-}	−1299.0	−1096.1
Dihydrogen phosphate	$H_2PO_4^-$	−1302.6	−1137.3
2-propanol	C_3H_8O	−330.8	−185.2
Pyrophosphate	$P_2O_7^{4-}$	−2293.5	−1919.9
	$HP_2O_7^{3-}$	−2294.9	−1973.9
	$H_2P_2O_7^{2-}$	−2295.4	−2012.2
	$H_3P_2O_7^-$	−2290.4	−2025.1
	$H_4P_2O_7$	−2281.2	−2029.9
Pyruvate	$C_3H_3O_3^-$	−596.2	−472.3
D-ribose	$C_5H_{10}O_5$	−1034.0	−738.8
D-ribose 5-phosphate	$C_5H_9O_8P^{2-}$	−2041.5	−1582.6
	$C_5H_{10}O_8P^-$	−2030.2	−1620.8
D-ribulose	$C_5H_{10}O_5$	−1023.0	−735.9
L-sorbose	$C_6H_{12}O_6$	−1263.3	−912.0
Succinate	$C_4H_4O_4^2-$	−908.7	−690.4
	$C_4H_5O_4^-$	−908.8	−722.6
	$C_4H_6O_4$	−912.2	−746.6
Sucrose	$C_{12}H_{22}O_{11}$	−2199.9	−1564.7
L-tryptophan	$C_{11}H_{12}N_2O_2$	−405.2	−114.7
Urea	CH_4N_2O	−317.7	−202.8
L-valine	$C_5H_{11}NO_2$	−612.0	−358.7
D-xylose	$C_5H_{10}O_5$	−1045.9	−750.5
D-xylulose	$C_5H_{10}O_5$	−1029.7	−746.2

*Estimated using data from R. N. Goldberg, Y. B. Tewari, and T. N. Bhat, *Thermodynamics of Enzyme Catalyzed Reactions*, NIST Standard Reference Database 74, http://xpdb.nist.gov/enzyme_thermodynamics.

†From Robert A. Alberty, *Thermodynamics of Biochemical Reactions*, Wiley-Interscience, Hoboken, NJ, USA, 2003. Table 3.2, pp. 52–55 and Table 8.2, p. 151.

Notes

1. The standard property changes of formation $\Delta H^\circ_{f_{298}}$ and $\Delta G^\circ_{f_{298}}$ 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), except as noted in Note 2.

2. Conventions used in this table are that $\Delta G^\circ_{f_{298}} = \Delta H^\circ_{f_{298}} = 0$ for H^+ and for oxidized nicotinamide-adenine dinucleotide $\left(NAD^-_{ox}\right)$. For the latter, and other NAD species, no molecular formula is provided because their properties are computed relative to this convention rather than relative to the elements in their standard states.