

APPENDIX A

Thermodynamic data (all values relate to 298.15 K and 1 bar of pressure)

Compound, Atom, or Ion	\bar{H}° or ΔH_f° (kJ mol ⁻¹)	μ° or \bar{G}_f° (kJ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	C_p° (J K ⁻¹ mol ⁻¹)
Aluminium				
Al(s)	0	0	28.33	24.35
Al(l)	10.56	7.20	39.55	24.21
Al(g)	326.4	285.7	164.54	21.38
Al ³⁺ (g)	5,483.17	—	—	—
Al ³⁺ (aq)	-531	-485	-321.7	—
Al ₂ O ₃ (s, α)	-1,675.7	-1,582.3	50.92	79.04
AlCl ₃ (s)	-704.2	-628.8	110.67	91.84
Argon				
Ar(g)	0	0	154.84	20.786
Antimony				
Sb(s)	0	0	45.69	25.23
SbH ₃ (g)	145.11	147.75	232.78	41.05
Arsenic				
As(s, α)	0	0	35.1	24.64
As(g)	302.5	261.0	174.21	20.79
As ₄ (g)	299.69	143.9	92.4	—
AsH ₃ (g)	66.44	68.93	222.78	38.07
Barium				
Ba(s)	0	0	62.8	28.07
Ba(g)	180	146	170.24	20.79
Ba ²⁺ (aq)	-537.64	-560.77	9.6	—
BaO(s)	-553.5	-525.1	70.43	47.78
BaCl ₂ (s)	-858.6	-810.4	123.68	75.14
Beryllium				
Be(s)	0	0	9.50	16.44
Be(g)	324.3	286.6	136.27	20.79
Bismuth				
Bi(s)	0	0	56.74	25.52
Bi(g)	207.1	168.2	187.00	20.79
Bromine				
Br ₂ (l)	0	0	152.23	75.689
Br ₂ (g)	30.907	3.110	245.46	36.02
Br(g)	111.88	82.396	175.02	20.786

Note: Dash indicates value of quantity unknown.

Compound, Atom, or Ion	\bar{H}° or ΔH_f° (kJ mol ⁻¹)	μ° or G_f° (kJ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	C_p° (J K ⁻¹ mol ⁻¹)
Br ⁻ (g)	-219.07	—	—	—
Br ⁻ (aq)	-121.55	-103.96	82.4	-141.8
HBr(g)	-36.40	-53.45	198.70	29.142
Cadium				
Cd(s, γ)	0	0	51.76	25.98
Cd(g)	112.01	77.41	167.75	20.79
Cd ²⁺ (aq)	-75.90	-77.612	-73.2	—
CdO(s)	-258.2	-228.4	54.8	43.43
CdCO ₃ (s)	-750.6	-669.4	92.5	—
Cesium				
Cs(s)	0	0	85.23	32.17
Cs(g)	76.06	49.12	175.60	20.79
Cs ⁺ (aq)	-258.28	-292.02	133.05	-10.5
Calcium				
Ca(s)	0	0	41.42	25.31
Ca(g)	178.2	144.3	154.88	20.786
Ca ²⁺ (aq)	-542.83	-553.58	-53.1	—
CaO(s)	-635.09	-604.03	39.75	42.80
CaCO ₃ (s) (calcite)	-1,206.9	-1,128.8	92.9	81.88
CaCO ₃ (s)	-1,207.1	-1,127.8	88.7	81.25
CaF ₂ (s)	-1,219.6	-1,167.3	68.87	67.03
CaCl ₂ (s)	-795.8	-748.1	104.6	72.59
CaBr ₂ (s)	-682.8	-663.6	130	—
Carbon				
C(s) (graphite)	0	0	5.740	8.527
C(s) (diamond)	1.895	2.900	2.377	6.113
C(g)	716.68	671.26	158.10	20.838
C ₂ (g)	831.90	775.89	199.42	43.21
CO(g)	-110.53	-137.17	197.67	29.14
CO ₂ (g)	-393.51	-394.36	213.74	37.11
H ₂ CO ₃ (aq)	-699.65	-623.08	187.4	—
HCO ₃ ⁻ (aq)	-691.99	-586.77	91.2	—
CO ₃ ²⁻ (aq)	-677.14	-527.81	-56.9	—
CCl ₄ (l)	-135.44	-65.21	216.40	131.75
CS ₂ (l)	89.70	65.27	151.34	75.7
HCN(g)	135.1	124.7	201.78	35.86
HCN(l)	108.87	124.97	112.84	70.63
CN ⁻ (aq)	150.6	172.4	94.1	—

Compound, Atom, or Ion	H° or ΔH_f° (kJ mol ⁻¹)	μ° or G_f° (kJ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	C_p° (J K ⁻¹ mol ⁻¹)
Organic Compounds				
Hydrocarbons				
CH ₄ (g) methane	-74.81	-50.72	186.26	35.31
CH ₃ (g) methyl	145.69	147.92	194.2	38.70
C ₂ H ₂ (g) ethyne	226.73	209.20	200.94	43.93
C ₂ H ₄ (g) ethene	52.26	68.15	219.56	43.56
C ₂ H ₆ (g) ethane	-84.68	-32.82	229.60	52.63
C ₃ H ₆ (g) propene	20.42	62.78	267.05	63.89
C ₃ H ₈ (g) propane	-103.85	-23.49	269.91	73.5
C ₃ H ₆ (g) cyclopropane	53.30	104.45	237.55	55.94
C ₄ H ₈ (g) 1-butene	-0.13	71.39	305.71	85.65
C ₄ H ₈ (g) <i>cis</i> -2-butene	-6.99	65.95	300.94	78.91
C ₄ H ₈ (g) <i>trans</i> -2-butene	-11.17	63.06	296.59	87.82
C ₄ H ₁₀ (g) butane	-126.15	-17.03	310.23	97.45
C ₅ H ₁₂ (g) pentane	-146.44	-8.20	348.40	120.2
C ₅ H ₁₂ (l) pentane	-173.1	—	—	—
C ₆ H ₆ (l) benzene	49.0	124.3	173.3	136.1
C ₆ H ₆ (g) benzene	82.93	129.72	269.31	81.67
C ₆ H ₁₂ (l) cyclohexane	-156	26.8	—	156.5
C ₆ H ₁₄ (l) hexane	-198.7	—	204.3	—
C ₇ H ₈ (g) toluene	50.0	122.0	320.7	103.6
C ₇ H ₁₆ (l) heptane	-224.4	1.0	328.6	224.3
C ₈ H ₁₈ (l) octane	-249.9	6.4	361.1	—
C ₈ H ₁₈ (l) isooctane	-255.1	—	—	—
C ₉ H ₂₀ (l) nonane	-288.1	—	—	284.4
C ₉ H ₂₀ (g) nonane	-228.2	—	—	—
C ₁₀ H ₈ (s) naphthalene	78.53	—	—	—
C ₁₀ H ₂₂ (l) decane	-300.9	—	—	314.4
C ₁₀ H ₂₂ (g) decane	-249.5	—	—	—
C ₁₁ H ₂₄ (l) undecane	-327.2	—	—	344.9
C ₁₁ H ₂₄ (g) undecane	-270.8	—	—	—
C ₁₂ H ₂₆ (l) dodecane	-350.9	—	—	375.8
C ₁₂ H ₂₆ (g) dodecane	-289.4	—	—	—
C ₁₄ H ₁₀ (s) anthracene	129.2	—	207.5	210.5
C ₆₀ (s) fullerene ₆₀	2,327.0	2,302.0	426.0	520.0
C ₆₀ (g) fullerene ₆₀	2,502.0	2,442.0	544.0	512.0
C ₇₀ (s) fullerene ₇₀	2,555.0	2,537.0	464.0	650.0
C ₇₀ (g) fullerene ₇₀	2,755.0	2,692.0	614.0	585.0
Alcohols and Phenols				
CH ₃ OH(l) methanol	-238.66	-166.27	126.8	81.6

Compound, Atom, or Ion	\bar{H}° or ΔH_f° (kJ mol ⁻¹)	μ° or \bar{G}_f° (kJ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	C_p^m (J K ⁻¹ mol ⁻¹)
CH ₃ OH(g)	-200.66	-161.96	239.81	43.89
C ₂ H ₅ OH(l) ethanol	-277.69	-174.78	160.7	111.46
C ₂ H ₅ OH(g)	-235.10	-168.49	282.70	65.44
C ₆ H ₅ OH(s) phenol	-165.0	-50.9	146.0	—
C ₃ H ₇ OH(l) 1-propanol	-302.6	—	193.6	143.9
C ₄ H ₉ OH(l) 1-butanol	-327.3	—	225.8	177.2
C ₅ H ₁₁ OH(l) 1-pentanol	-351.6	—	—	208.1
C ₆ H ₁₃ OH(l) 1-hexanol	-377.5	—	287.4	240.4
C ₇ H ₁₅ OH(l) 1-heptanol	-403.3	—	—	272.1
C ₈ H ₁₇ OH(l) 1-octanol	-426.5	—	—	305.2
C ₉ H ₁₉ OH(l) 1-nonanol	-453.4	—	—	—
C ₁₀ H ₂₁ OH(l) 1-decanol	-478.1	—	—	370.6
Carboxylic Acids and Esters				
HCO ₂ H(l) formic	-424.72	-361.35	128.95	99.04
CH ₃ CO ₂ H(l) acetic	-484.5	-389.9	159.8	124.3
CH ₃ CO ₂ H(aq)	-485.76	-396.46	178.7	—
CH ₃ CO ₂ ⁻ (aq)	-486.01	-369.31	86.6	-6.3
(CO ₂ H) ₂ (s) oxalic	-827.2	—	—	117
C ₆ H ₅ CO ₂ (s) benzoic	-385.1	-245.3	167.6	146.8
CH ₃ CO ₂ C ₂ H ₅ (l) ethyl acetate	-479.0	-332.7	259.4	170.1
Aldehydes and Ketones				
HCHO(g) methanal	-108.57	-102.53	218.77	35.40
CH ₃ CHO(l) ethanal	-192.30	-128.12	160.2	—
CH ₃ CHO(g)	-166.19	-128.86	250.3	57.3
CH ₃ COCH ₃ (l) propanone	-248.1	-155.4	200.4	124.7
C ₂ H ₅ CHO(l) propanal	-215.6	—	—	—
C ₂ H ₅ CHO(g)	-185.6	—	304.5	80.7
C ₃ H ₇ CHO(l) butanal	-239.2	—	246.6	163.7
C ₃ H ₇ CHO(g)	-204.8	—	343.7	103.4
C ₂ H ₅ COCH ₃ (l) butanone	-273.3	—	239.1	158.7
C ₂ H ₅ COCH ₃ (g)	-238.5	—	339.9	101.7
Sugars				
C ₆ H ₁₂ O ₆ (s) α-D-glucose	-1,273.3	—	—	—
C ₆ H ₁₂ O ₆ (s) β-D-glucose	-1,286	-910	212	—
C ₆ H ₁₂ O ₆ (s) β-D-fructose	-1,265.6	—	—	—
C ₁₂ H ₂₂ O ₁₁ (s) sucrose	-2,222	-1,543	360.2	—

Compound, Atom, or Ion	\bar{H}° or ΔH_f° (kJ mol ⁻¹)	μ° or \bar{G}_f° (kJ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	C_p° (J K ⁻¹ mol ⁻¹)
Nitrogen Compounds				
CO(NH ₂) ₂ (s) urea	-333.51	-197.33	104.60	93.14
CH ₃ NH ₂ (g) methyl amine	-22.97	32.16	243.41	53.1
C ₆ H ₅ NH ₂ (l) aniline	31.1	—	—	—
Ethers				
CH ₃ OC(CH ₃) ₃ (l) methyl <i>tert</i> -butyl ether (MTBE)	-313.6	—	265.3	187.5
CH ₃ OC(CH ₃) ₃ (g)	-283.7	—	—	—
Chlorine				
Cl ₂ (g)	0	0	223.07	33.91
Cl(g)	121.68	105.68	165.20	21.840
Cl ⁻ (g)	-233.13	—	—	—
Cl ⁻ (aq)	-167.16	-131.23	56.5	-136.4
HCl(g)	-92.31	-95.30	186.91	29.12
HCl(aq)	-167.16	-131.23	56.5	-136.4
Chromium				
Cr(s)	0	0	23.77	23.35
Cr(g)	396.6	351.8	174.50	20.79
CrO ₄ ²⁻ (aq)	-881.15	-727.75	50.21	—
Cr ₂ O ₇ ²⁻ (aq)	-1,490.3	-1,301.1	261.9	—
Copper				
Cu(s)	0	0	33.150	23.35
Cu(g)	338.32	298.58	166.38	20.79
Cu ⁺ (aq)	71.67	49.98	40.6	—
Cu ²⁺ (aq)	64.77	65.49	-99.6	—
Cu ₂ O(s)	-168.6	-146.0	93.14	63.64
CuO(s)	-157.3	-129.7	42.63	42.30
CuSO ₄ (s)	-771.36	-661.8	109	100.0
Deuterium				
D ₂ (g)	0	0	144.96	29.20
HD(g)	0.318	-1.464	143.80	29.196
D ₂ O(g)	-249.20	-234.54	198.34	34.27
D ₂ O(l)	-294.60	-243.44	75.94	84.35
HDO(g)	-245.30	-233.11	199.51	33.81
HDO(l)	-289.89	-241.86	79.29	—
Fluorine				
F ₂ (g)	0	0	202.78	31.30
F(g)	78.99	61.91	158.75	22.74

Compound, Atom, or Ion	\bar{H}° or ΔH_f° (kJ mol ⁻¹)	$\bar{\mu}^\circ$ or G_f° (kJ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	C_p° (J K ⁻¹ mol ⁻¹)
F ⁻ (aq)	-332.63	-278.79	-13.8	-106.7
HF(g)	-271.1	-273.2	173.78	29.13
Helium				
He(g)	0	0	126.15	20.786
Hydrogen				
H ₂ (g)	0	0	130.684	28.824
H(g)	217.97	203.25	114.71	20.784
H ⁺ (aq)	0	0	0	0
H ₂ O(l)	-285.83	-237.13	69.91	75.291
H ₂ O(g)	-241.82	-228.57	188.83	33.58
H ₂ O ₂ (l)	-187.78	-120.35	109.6	89.1
Iodine				
I ₂ (s)	0	0	116.135	54.44
I ₂ (g)	62.44	19.33	260.69	36.90
I(g)	106.84	70.25	180.79	20.786
I ⁻ (aq)	-55.19	-51.57	111.3	-142.3
HI(g)	26.48	1.70	206.59	29.158
Iron				
Fe(s)	0	0	27.28	25.10
Fe(g)	416.3	370.7	180.49	25.68
Fe ²⁺ (aq)	-89.1	-78.90	-137.7	—
Fe ³⁺ (aq)	-48.5	-4.7	-315.9	—
Fe ₃ O ₄ (s)	-1,118.4	-1,015.4	146.4	143.43
Fe ₂ O ₃ (s)	-824.2	-742.2	87.40	103.85
FeS(s)	-100.0	-100.4	60.29	50.54
Krypton				
Kr(g)	0	0	164.08	20.786
Lead				
Pb(s)	0	0	64.81	26.44
Pb(g)	195.0	161.9	175.37	20.79
Pb ²⁺ (aq)	-1.7	-24.43	10.5	—
PbO(s) yellow	-217.32	-187.89	68.70	45.77
PbO(s) red	-218.99	-188.93	66.5	45.81
PbO ₂ (s)	-277.4	-217.33	68.6	64.64
Lithium				
Li(s)	0	0	29.12	24.77
Li(g)	159.37	126.66	138.77	20.79
Li ⁺ (aq)	-248.49	-293.31	13.4	68.6
Magnesium				
Mg(s)	0	0	32.68	24.89
Mg(g)	147.70	113.10	148.65	20.786
Mg ²⁺ (aq)	-466.85	-454.8	-138.1	—

Compound, Atom, or Ion	\bar{H}° or ΔH_f° (kJ mol ⁻¹)	$\bar{\mu}^\circ$ or \bar{G}_f° (kJ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	C_p° (J K ⁻¹ mol ⁻¹)
MgO(s)	-601.70	-569.43	26.94	37.15
MgCO ₃ (s)	-1,095.8	-1,012.1	65.7	75.52
MgCl ₂ (s)	-641.32	-591.79	89.62	71.38
Mercury				
Hg(l)	0	0	76.02	27.983
Hg(g)	61.32	31.82	174.96	20.786
Hg ²⁺ (aq)	171.1	164.40	-32.2	—
Hg ₂ ²⁺ (aq)	172.4	153.52	84.5	—
HgO(s)	-90.83	-58.54	70.29	44.06
Hg ₂ Cl ₂ (s)	-265.22	-210.75	192.5	102
HgCl ₂ (s)	-224.3	-178.6	146.0	—
HgS(s)	-53.6	-47.7	88.3	—
Neon				
Ne(g)	0	0	146.33	20.786
Nitrogen				
N ₂ (g)	0	0	191.61	29.125
N(g)	472.70	455.56	153.30	20.786
NO(g)	90.25	86.55	210.76	29.844
N ₂ O(g)	82.05	104.20	219.85	38.45
NO ₂ (g)	33.18	51.31	240.06	37.20
N ₂ O ₄ (g)	9.16	97.89	304.29	77.28
N ₂ O ₅ (s)	-43.1	113.9	178.2	143.1
N ₂ O ₅ (g)	11.3	115.1	355.7	84.5
HNO ₃ (l)	-174.10	-80.71	155.60	109.87
HNO ₃ (aq)	-207.36	-111.25	146.4	-86.6
NO ₃ ⁻ (aq)	-205.0	-108.74	146.4	-86.6
NH ₃ (g)	-46.11	-16.45	192.45	35.06
NH ₃ (aq)	-80.29	-26.50	111.3	—
NH ₄ ⁺ (aq)	-132.51	-79.31	113.4	79.9
HN ₃ (l)	264.0	327.3	140.6	43.68
HN ₃ (g)	294.1	328.1	238.97	98.87
N ₂ H ₄ (l)	50.63	149.43	121.21	139.3
NH ₄ NO ₃ (s)	-365.56	-183.87	151.08	84.1
NH ₄ Cl(s)	-314.43	-202.87	94.6	—
Oxygen				
O ₂ (g)	0	0	205.138	29.355
O(g)	249.17	231.73	161.06	21.912
O ₃ (g)	142.7	163.2	238.93	39.20
OH ⁻ (aq)	-229.99	-157.24	-10.75	-148.5
Phosphorus				
P(s) white	0	0	41.09	23.840

Compound, Atom, or Ion	\bar{H}° or ΔH_f° (kJ mol ⁻¹)	μ° or \bar{G}_f° (kJ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	C_p° (J K ⁻¹ mol ⁻¹)
P(g)	314.64	278.25	163.19	20.786
P ₂ (g)	144.3	103.7	218.13	32.05
P ₄ (g)	58.91	24.44	279.98	67.15
PH ₃ (g)	5.4	13.4	210.23	37.11
PCl ₃ (g)	-287.0	-267.8	311.78	71.84
PCl ₅ (g)	-374.9	-305.0	364.6	112.8
H ₃ PO ₃ (s)	-964.4	—	—	—
H ₃ PO ₃ (aq)	-964.8	—	—	—
H ₃ PO ₄ (s)	-1,279.0	-1,119.1	110.50	106.06
H ₃ PO ₄ (l)	-1,266.9	—	—	—
H ₃ PO ₄ (aq)	-1,277.4	-1,018.7	-222	—
PO ₄ ³⁻ (aq)	-2,984.0	-2,697.0	228.86	211.71
Potassium				
K(s)	0	0	64.18	29.58
K(g)	89.24	60.59	160.336	20.786
K ⁺ (g)	514.26	—	—	—
K ⁺ (aq)	-252.38	-283.27	102.5	21.8
KOH(s)	-424.76	-379.08	78.9	64.9
KF(s)	-576.27	-537.27	66.57	49.04
KCl(s)	-436.75	-409.14	82.59	51.30
KBr(s)	-393.80	-380.66	95.90	52.30
KI(s)	-327.90	-324.89	106.32	52.93
Silicon				
Si(s)	0	0	18.83	20.00
Si(g)	455.6	411.3	167.97	22.25
SiO ₂ (s)	-910.94	-856.64	41.84	44.43
Silver				
Ag(s)	0	0	42.55	25.351
Ag(g)	284.55	245.65	173.00	20.79
Ag ⁺ (aq)	105.58	77.11	72.68	21.8
AgBr(s)	-100.37	-96.90	107.1	52.38
AgCl(s)	-127.07	-109.79	96.2	50.79
Ag ₂ O(s)	-31.05	-11.20	121.3	65.86
AgNO ₃ (s)	-124.39	-33.41	140.92	93.05
Sodium				
Na(s)	0	0	51.21	28.24
Na(g)	107.32	76.76	153.71	20.79
Na ⁺ (aq)	-240.12	-261.91	59.0	46.4
NaOH(s)	-425.61	-379.49	64.46	59.54
NaCl(s)	-411.15	-384.14	72.13	50.50
NaBr(s)	-361.06	-348.98	86.82	51.38

Compound, Atom, or Ion	H° or ΔH_f° (kJ mol ⁻¹)	μ° or G_f° (kJ mol ⁻¹)	S° (J K ⁻¹ mol ⁻¹)	C_p° (J K ⁻¹ mol ⁻¹)
NaI(s)	-287.78	-286.06	98.53	52.09
Sulfur				
S(s) rhombic	0	0	31.80	22.64
S(s) monoclinic	0.33	0.1	32.6	23.6
S(g)	278.81	238.25	167.82	23.673
S ₂ (g)	128.37	79.30	228.18	32.47
SO ₂ (g)	-296.83	-300.19	248.22	39.87
SO ₃ (g)	-395.72	-371.06	256.76	50.67
H ₂ SO ₄ (l)	-813.99	-690.00	156.90	138.9
H ₂ SO ₄ (aq)	-909.27	-744.53	20.1	-293
SO ₄ ²⁻ (aq)	-909.27	-744.53	20.1	-293
HSO ₄ ⁻ (aq)	-887.34	-755.91	131.8	-84
H ₂ S(g)	-20.63	-33.56	205.79	34.23
H ₂ S(aq)	-39.7	-27.83	121	—
HS ⁻ (aq)	-17.6	12.08	62.08	—
SF ₆ (g)	-1,209	-1,105.3	291.82	97.28
Tin				
Sn(s)	0	0	51.55	26.99
Sn(g)	302.1	267.3	168.49	20.26
Sn ²⁺ (aq)	-8.8	-27.2	-17	—
SnO(s)	-285.8	-256.9	56.5	44.31
SnO ₂ (s)	-580.7	-519.6	52.3	52.59
Xenon				
Xe(g)	0	0	169.68	20.786
Zinc				
Zn(s)	0	0	41.63	25.40
Zn(g)	130.73	95.14	160.98	20.79
Zn ²⁺ (aq)	-153.89	-147.06	112.1	46
ZnO(s)	-348.28	-318.30	43.64	40.25

Sources of data: *Handbook of Chemistry and Physics*, 78th ed., CRC Press, Boca Raton, FL, 1997–1998. P. Atkins, *Physical Chemistry*, 5th ed., New York: W. H. Freeman and Co., 1994.