TABLE 15. *Gibbs free energies of formation from the elements for compounds of biological interest*[a]

Substance	State	$-\Delta Gf^{\circ}$ (25°C)		References
		kcal/mol	kJ/mol	
H_2	g	0	0	683
H^+	aq	0	0	683
H^+ (pH 7)	aq	9.53	39.87	See text
H_2O	liq	56.687	237.178	683
HO^-	aq	37.594	157.293	683
H_2O_2	aq	32.05	134.097	683
O_2^-	aq	[−6.9]	[−28.9]	—[b]
C graphite	c	0		683
CO	g	32.78	137.15	683
CO_2	g	94.254	394.359	683
	aq	92.26	386.02	683
H_2CO_3	aq	148.94	623.16	683
HCO_3^-	aq	140.26	586.85	683
CO_3^{2-}	aq	126.17	527.90	683
Hydrocarbons				
CH_4	g	12.13	50.75	683
C_2H_6	g	7.86	32.89	683
C_2H_4	g	−16.28	−68.12	683
C_2H_2	g	−50.00	−209.2	683
Alcohols				
Methanol	aq	41.92	175.39	683
Ethanol	aq	43.44	181.75	683
n-Propanol	aq	42.02	175.81	91
iso-Propanol	aq	44.44	185.94	91, 94
n-Butanol	aq	41.07	171.84	91, 92
Ethylene glycol	liq	77.25	323.21	683
	aq	[79]	[330.5]	618
Glycerol	liq	114.02	477.06	91, 92
	aq	116.76	488.52	91, 92
Mannitol	aq	225.29	942.61	91
Sorbitol	aq	225.31	942.70	91
Aldehydes:				
Formaldehyde	aq	31.2	130.54	91
	g	27	112.97	683
Acetaldehyde	aq	33.4	139.9	—[c]
	g	30.81	128.91	683
Butyraldehyde	liq	28.6	119.67	303
Ketones:				
Acetone	aq	38.52	161.17	91, 92
Monocarboxylic acids				
Formate$^-$	aq	83.9	351.04	683[n]
Acetate$^-$	aq	88.29	369.41	683
Propionate$^-$	aq	[86.3]	[361.08]	618
Butyrate$^-$	aq	84.28	352.63	91, 92
Valerate$^-$	aq	[82.3]	[344.34]	—[d]
Caproate$^-$	aq	[80.3]	[335.96]	—[d]
Palmitic acid	c	72.9	305.0	345
Acrylate$^-$	aq	[68.4]	[286.19]	—[e]
Crotonate$^-$	aq	66.3	277.4	—[f]
Glycollate$^-$	aq	126.9	530.95	91
Lactate$^-$	aq	123.6	517.81	91, 92
β-Hydroxypropionate	aq	123.9	518.4	618
β-Hydroxybutyrate	aq	[121]	[506.3]	91
Glycerate$^-$	aq	[157.3]	[658.1]	—[g]
D-Gluconate$^-$	aq	[269.7]	[1128.3]	—[h]
Glyoxylate$^-$	aq	112.0	468.6	91, 282
Pyruvate$^-$	aq	113.44	474.63	91, 92
β-Ketobutyrate$^-$	aq	118	493.7	91[o]
Dicarboxylic-acid				
Oxalate^{1-}	aq	166.93	698.44	683

TABLE 15—*Continued*

Substance	State	$-\Delta Gf^\circ$ (25°C)		References
		kcal/mol	kJ/mol	
Oxalate^{2-}	aq	161.1	674.04	683
Succinic acid	aq	178.39	746.38	91, 92
Succinate^{2-}	aq	164.97	690.23	91, 92
Fumaric acid	aq	154.67	647.14	91, 92
Fumarate^{2-}	aq	144.41	604.21	91, 92
L-Malate^{2-}	aq	201.98	845.08	91, 92
Oxalacetate^{2-}	aq	190.53	797.18	91, 92
α-ketoglutarate	aq	190.62	797.55	91, 92
Tricarboxylic acids				
Citrate^{3-}	aq	279.24	1,168.34	91, 90
Isocitrate^{3-}	aq	277.65	1,161.69	91, 90
cis-Aconitate^{3-}	aq	220.51	922.61	91, 90
Carbohydrates:				
Glyceraldehyde	aq	[104.6]	[437.65]	—[i]
Dihydroxyacetone	aq	[106.5]	[445.18]	—[j]
D-Erythrose	aq	[143.]	[598.3]	—[k]
D-Ribose	aq	[181]	[757.3]	—[k]
α-D-Glucose	aq	219.22	917.22	91, 92
α-D-Galactose	aq	220.73	923.53	91
D-Fructose	aq	218.78	915.38	91
D-Heptose	aq	[257]	[1,077]	—[k]
α-Lactose	aq	362.15	1,515.24	91, 92
β-Lactose	aq	375.26	1,570.09	91, 92
β-Maltose	aq	357.80	1,497.04	91, 92
Sucrose	aq	370.90	1,551.85	91, 92
Glycogen (per unit of glucose)	aq	158.3	662.33	91
Amino acids				
L-Alanine	aq	88.8	371.54	92, 260
L-Arginine	c	57.4	240.2	91, 260
L-Asparagine × H_2O	aq	182.6	763.998	92, 260
L-Aspartic acid	aq	172.4	721.3	92, 260
L-Aspartate$^-$	aq	167.14	700.4	—[l]
L-Cysteine	aq	81.21	339.78	91
L-Cystine	aq	159.4	666.93	260
L-Glutamic acid	aq	173.0	723.8	260
L-Glutamate$^-$	aq	167.2	699.6	—[m]
L-Glutamine	aq	126.6	529.7	260
Glycine	aq	88.618	370.788	683
Glycine$^+$	aq	91.824	384.192	683
Glycine$^-$	aq	75.278	314.963	683
L-Leuine	aq	82.0	343.1	91, 260
L-Isoleucine	aq	82.2	343.9	260
L-Methionine	aq	120.2	502.92	260
L-Phenylalanine	aq	49.5	207.1	260
L-Serine	aq	122.1	510.87	260
L-Threonine	aq	[123]	[514.63]	260
	c	131.5	550.2	
L-Tryptophane	aq	26.9	112.6	260
L-Tyrosine	aq	88.6	370.7	260
L-Valine	aq	85.3	356.9	260
Purines				
Hypoxanthine	aq	−21.4	−89.5	91
Guanine	c	−11.23	−46.99	91
Xanthine	c	39.64	165.85	91
Urate$^-$	aq	77.9	325.9	91
Uric acid	aq	85.3	356.9	91
Other N-containing compounds				
Urea	c	47.04	196.82	683
	aq	48.7	203.76	683
Creatine	aq	63.17	264.30	91

TABLE 15—*Continued*

Substance	State	$-\Delta Gf°$ (25°C)		References
		kcal/mol	kJ/mol	
Creatinine	aq	6.91	28.91	91
Allantoin	c	106.62	446.098	91
NH_2-CH_2-CH_2-SO_3^-	aq	121.76	509.4	683
$CH_3NH_3^+$	aq	9.55	40.0	683
$(CH_3)_2NH_2^+$	aq	0.8	3.3	683
$(CH_3)_3NH^+$	aq	−8.9	−37.2	683
Pyridine		−42.33	−177.1	303
Aromatic compounds				
Benzene		−29.76	−124.5	303
Phenol	c	11.38	47.6	303
		12.45	52.1	
p-Quinone	c	20.0	83.7	303
p-Hydroquinone	c	49.48	207.0	303
Resorcinol	c	50.00	209.2	303
Pyrocatechol	c	50.20	210.0	303
o-Cresol	g	8.86	37.1	303
m-Cresol	g	9.69	40.54	303
p-Cresol	g	7.67	32.09	303
Toluene	liq	−27.30	−114.22	303
Benzoic acid	c	58.7	245.6	303
		59.4	248.5	
o-Hydroxybenzoic acid	c	100.7	421.33	303
m-Hydroxybenzoic acid	c	101.0	422.58	303
p-Hydroxybenzoic acid	c	101.1	423.00	303
Benzyl alcohol	liq	7.47	31.25	303
		6.6	27.6	
N_2	g	0		683
NH_3	aq	6.35	26.57	683
NH_4^+	aq	18.97	79.37	683
NO	g	−20.69	−86.57	683
NO_2^-	aq	8.9	37.2	683
NO_3^-	aq	26.61	111.34	683
N_2O	g	−24.90	−104.18	683
N_2H_4	aq	−30.6	−128.03	683
ClO_2^-	aq	−4.1	−17.2	683
ClO_3^-	aq	0.8	3.35	683
S rhombic	c	0		683
S^{2-}	aq	−20.5	−85.8	683
SH^-	aq	−2.88	−12.05	683
SH_2	g	8.02	33.56	683
	aq	6.66	27.87	683
SO_3^{2-}	aq	116.3	486.6	683
HSO_3^-	aq	126.15	527.81	683
H_2SO_3	aq	128.56	537.895	683
SO_2	g	71.748	300.194	683
	aq	71.871	300.708	683
SO_4^{2-}	aq	177.97	744.63	683
SO_4H^-	aq	180.69	756.01	683
$S_2O_3^{2-}$	aq	122.7	513.4	406
$S_2O_4^{2-}$	aq	143.5	600 4	683
$HS_2O_4^-$	aq	146.9	614.6	683
$S_3O_6^{2-}$	aq	229	958.1	349, 546
$S_4O_6^{2-}$	aq	244.3	1,022.2	349
$H_2S_2O_4$	aq	147.4	616.7	683
Fe^{2+}	aq	18.85	78.87	684
Fe^{3+}	aq	1.1	4.6	684

[a] The table is a revision of the table published by Burton in 1957 (91). It contains the revised free energies of formation for C_1 and C_2 compounds of Technical Note 270-3 of the National Bureau of Standards issued in 1968 (683), and the newly determined values for amino acids of Hutchens of 1970 (260). In addition, this table contains free energies of formation of a series of inorganic compounds previously not thought to be of biological interest. The physical state of each substance is indicated in the column headed "State" as cristalline solid (c), liquid (liq), or gaseous (g). Solutions in water are listed as aqueous (aq). The values in parentheses have been obtained by approximate calculation.

TABLE 15—*Continued*

[b] Calculated from E_0 (O_2/O_2^-) = −300 mV (559).

[c] Calculated from ΔGf^0 for ethanol and E_0' (acetaldehyde/ethanol) = −200 mV (91).

[d] Calculated assuming that per CH_2 group, ΔGf^0 decreases by 2 kcal/mol from acetate to caproate.

[e] Calculated from ΔGf^0 for propionate and E_0' (crotonate/butyrate) = −25 mV (232).

[f] Calculated from ΔGf^0 for butyrate and E_0' (crotonate/butyrate) = −25 mV (232).

[g] Calculated from ΔGf^0 for glyceraldehyde and $\Delta G^{0\prime}$ (glyceraldehyde-phosphate + $H_2O \rightarrow$ phosphoglycerate$^-$ + H^+ + H_2) = −5.4 kcal/mol (679; see also 91, 334).

[h] Calculated from ΔGf^0 for glucose and $\Delta G^{0\prime}$ (glucose + $H_2O \rightarrow$ gluconate$^-$ + H^+ + H_2) = −3.36 kcal/mol (384).

[i] Calculated from ΔGf^0 for dihydroxyacetone and $\Delta G^{0\prime}$ (dihydroxyacetone-phosphate → glyceraldehyde-phosphate) = +1.83 kcal/mol (91).

[j] Calculated from ΔGf^0 for glycerol and E_0' (dihydroxyacetone phosphate/glycerolphosphate) = −190 mV (91).

[k] Calculated assuming that per CH_2OH group, ΔGf^0 increases by 38.2 kcal/mol.

[l] Calculated from DGf^0 and pK_a (=3.65) for aspartic acid (ΔGf^0 [dissociation] = 2.3 RT pK).

[m] Calculated from ΔGf^0 and pK_a (=4.25) for glutamic acid.

[n] A ΔGf^0 of −80 kcal/mol has been reported for formate by Latimer (349).

[o] A ΔGf^0 of 114.1 kcal/mol is obtained if an E_0' (β-keto butyrate/β-hydroxybutyrate) of −270 mV (384) instead −349 mV (91) is used to calculate ΔGf^0 for β-ketobutyrate from ΔGf^0 for β-hydroxybutyrate.