

# A Thermochemical Data

The data in this appendix have been compiled from a number of sources. Nearly all of the critical property data are taken from Appendix A of *The Properties of Gases and Liquids*, Second Edition, by R. C. Reid and T. K. Sherwood, copyright © 1966, McGraw-Hill Book Company. They are used with the permission of McGraw-Hill Book Company. Most of the thermochemical data ( $\Delta G_f^\circ$ ,  $\Delta H_f^\circ$ , and  $S^\circ$ ) were obtained from the following sources.

1. Zwolinski, B. J., et al., "Selected Values of Properties of Hydrocarbons and Related Compounds," American Petroleum Institute Research Project 44, Thermodynamics Research Center, Texas A & M University,

College Station, Texas (Loose-leaf data sheets, extant, 1977).

2. Zwolinski, B. J., et al., "Selected Values of Properties of Chemical Compounds," Thermodynamics Research Center Data Project, Thermodynamics Research Center, Texas A & M University, College Station, Texas (Loose-Leaf data sheets, extant, 1977).

They are used with permission of the Thermodynamics Research Center. Other sources used include the *Handbook of Chemistry and Physics*, 57th edition, edited by R. C. Weast, CRC Press, Cleveland, 1974; and *Lange's Handbook of Chemistry*, 11th edition, edited by J. A. Dean, McGraw-Hill Book Company, New York, 1973.

Compound	State of aggregation	Molecular weight	$\Delta G_f^\circ$ , kcal/g-mole	$\Delta H_f^\circ$ , kcal/g-mole	$S_{25^\circ\text{C}}^\circ$ Absolute entropy cal/g-mole-°K	$T_c$ °K	$P_c$ Atm
Elementary gases							
Hydrogen	Gas	2.016	0	0	31.211	33.3	12.80
Oxygen	Gas	32.000	0	0	49.003	154.8	50.1
Nitrogen	Gas	28.016	0	0	45.767	126.2	33.5
Fluorine	Gas	38.00	0	0	48.6	144.	55.
Chlorine	Gas	70.91	0	0	53.286	417.	76.1
Bromine	Liquid	159.83	0	0	36.4	584.	102.
Iodine	Crystal	253.82	0	0	27.9	785.	116.
Paraffins							
Methane	Gas	16.04	- 12.140	- 17.889	44.50	190.7	45.8
Ethane	Gas	30.07	- 7.860	- 20.236	54.85	305.4	48.2
Propane	Gas	44.09	- 5.614	- 24.820	64.51	369.9	42.0
<i>n</i> -Butane	Gas	58.12	- 4.10	- 30.15	74.12	425.2	37.5
Isobutane	Gas	58.12	- 5.00	- 32.15	70.42	408.1	36.0
<i>n</i> -Pentane	Gas	72.15	- 2.00	- 35.00	83.40	469.5	33.3
2-Methylbutane	Gas	72.15	- 3.50	- 36.92	82.12	460.4	32.9
Neopentane	Gas	72.15	- 3.64	- 39.67	73.23	433.8	31.6
<i>n</i> -Hexane	Gas	86.17	- 0.07	- 39.96	92.83	507.3	29.9
2-Methylpentane	Gas	86.17	- 1.20	- 41.66	90.95	496.5	30.0
3-Methylpentane	Gas	86.17	- 0.51	- 41.02	90.77	504.7	30.8

Compound	State of aggregation	Molecular weight	$\Delta G_{f,25}^{\circ}$ kcal/g-mole	$\Delta H_{f,25}^{\circ}$ kcal/g-mole	$S_{25}^{\circ}$ Absolute entropy cal/g-mole-°K	$T_c$ °K	$P_c$ Atm
<b>Olefins</b>							
Ethylene	Gas	28.05	16.282	12.496	52.45	283.1	50.5
Propene	Gas	42.08	14.990	4.879	63.80	365.1	45.4
1-Butene	Gas	56.10	17.09	- 0.03	73.04	419.6	39.7
<i>cis</i> -2-Butene	Gas	56.10	15.74	- 1.67	71.90	434.6	40.5
<i>trans</i> -2-Butene	Gas	56.10	15.05	- 2.67	70.86	428.6	41.5
Isobutylene	Gas	56.10	13.88	- 4.04	70.17	419.7	39.5
1-Pentene	Gas	70.13	18.96	- 5.00	82.65	464.8	39.9
<i>cis</i> -2-Pentene	Gas	70.13	17.17	- 6.71	82.76	475.6	40.4
<i>trans</i> -2-Pentene	Gas	70.13	16.76	- 7.59	81.36	475.6	40.4
3-Methyl-1-butene	Gas	70.13	17.87	- 6.92	79.70	464.8	33.9
2-Methyl-2-butene	Gas	70.13	14.26	- 10.17	80.92	470.	34.
1-Hexene	Gas	84.16	20.94	- 9.96	91.93	504.0	31.1 <sup>a</sup>
1-Octene	Gas	112.21	24.96	- 19.82	110.55	578.	25.5 <sup>a</sup>
Cyclopentene	Gas	68.11	26.48	7.87	69.23	506.1	47.2 <sup>a</sup>
<b>Diolefins</b>							
Propadiene	Gas	40.06	48.37	45.92	58.30	393.3	43.6 <sup>a</sup>
1,3-Butadiene	Gas	54.09	36.43	26.75	66.62	425.	42.7
<b>Acetylenes</b>							
Acetylene	Gas	26.04	50.000	54.194	47.997	309.5	61.6
Propyne	Gas	40.06	46.313	44.319	59.30	401.	52.8
Ethylacetylene	Gas	54.09	48.30	39.48	69.51	463.7	37.5 <sup>a</sup>
Dimethylacetylene	Gas	54.09	44.32	34.97	67.71	488.7	37.5 <sup>a</sup>
<b>Cycloparaffins</b>							
Cyclopentane	Gas	70.13	9.29	- 18.41	70.00	511.8	44.6
Methylcyclopentane	Gas	84.16	8.55	- 25.50	81.24	532.7	37.4
Ethylcyclopentane	Gas	98.18	10.66	- 30.37	90.42	569.5	33.5
Cyclohexane	Gas	84.16	7.60	- 29.43	71.28	553.2	40.
Methylcyclohexane	Gas	98.18	6.52	- 36.99	82.06	572.1	34.3
<b>Aromatics</b>							
Benzene	Gas	78.11	30.989	19.820	64.34	562.1	48.6
Toluene	Gas	92.13	29.228	11.950	76.42	592.0	41.6
<i>o</i> -Xylene	Gas	106.16	29.177	4.540	84.31	631.6	35.7
<i>m</i> -Xylene	Gas	106.16	28.405	4.120	85.49	616.8	34.7
<i>p</i> -Xylene	Gas	106.16	28.952	4.290	84.23	618.8	33.9
Ethylbenzene	Gas	106.16	31.208	7.120	86.15	617.1	36.9
<b>Alcohols</b>							
Methyl alcohol	Gas	32.04	- 38.81	- 48.05	57.29	513.2	78.5
	Liquid		- 39.85	- 57.11	30.4		
Ethyl alcohol	Gas	46.07	- 40.13	- 56.03	67.54	516.3	63.0
	Liquid		- 41.65	- 66.20	38.53		

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<i>n</i> -Propyl alcohol	Gas	60.09	- 38.75	- 61.33	77.70	536.7	51.0
	Liquid		- 40.94	- 72.66	47.0		
Isopropyl alcohol	Gas	60.09	- 41.44	- 65.08	74.1	508.2	47.0
	Liquid		- 43.10	- 75.98	43.15		
<i>n</i> -Butyl alcohol	Gas	74.12	- 36.11	- 65.65	86.92	563.0	43.6
	Liquid		- 39.00	- 78.18	54.5		
<i>sec</i> -Butyl alcohol	Gas	74.12	- 42.33	- 70.00	85.8	536.0	41.4
	Liquid		- 40.12	- 81.86	53.4		
<i>tert</i> -Butyl alcohol	Gas	74.12	- 42.45	- 74.68	77.92	506.2	39.2
Isobutyl alcohol	Gas	74.12	- 40.12	- 70.00	85.8	547.7	42.4
	Liquid		- 42.33	- 81.06	53.4		
Phenol	Gas	94.11	- 7.61	- 22.98	75.43	694.3	60.5
	Liquid		- 12.17	- 39.44	34.9		
Ethers							
Dimethylether	Gas	46.07	- 26.96	- 43.99	63.74	400.1	52.6
Diethylether	Liquid	74.12	- 29.32	- 66.83	60.2	465.8	35.6
Isopropylether	Gas	102.17	- 28.5	- 76.24	91.2	500.1	28.4
	Liquid		- 30.09	- 84.00	70.4		
Ketones							
Acetone	Gas	58.08	- 36.50	- 51.79		509.1	47.
	Liquid		- 37.22	- 59.32			
Aldehydes							
Formaldehyde	Gas	30.03	- 27	- 28	52.26		
Acetaldehyde	Gas	44.05	- 30.81	- 39.72	59.8	461.	54.7 <sup>a</sup>
Organic Acids							
Acetic acid	Liquid	60.05	- 93.8	- 116.4	38.2	594.8	57.1
	Gas		- 91.24	- 104.72			
Acetic anhydride	Gas	102.09	- 119.29	- 148.82		569.2	46.2
	Liquid		- 121.75	- 155.16			
Propionic acid	Gas	74.08	- 88.27	- 108.75		612.7	53.0
	Liquid		- 91.65	- 121.7			
Esters							
Methyl formate	Gas	60.05	- 71.37	- 83.7	29	487.2	59.2
	Liquid		- 71.53	- 90.60			
Ethyl acetate	Gas	88.10	- 74.93	- 102.02		523.3	37.8
	Liquid		- 76.11	- 110.72			
Ethyl propionate	Gas	102.13	- 77.37	- 112.36		546.1	33.0
	Liquid		- 79.16	- 122.16			
Nitrogen compounds							
Ammonia	Gas	17.03	- 3.94	- 11.02	45.97	405.6	112.5
Cyanogen	Gas	52.02	70.81	73.60	57.86	400.	60.0
Hydrogen cyanide	Gas	27.03	28.7	31.2	48.23	456.7	48.9
Methyl amine	Gas	31.06	+ 6.6	- 6.7	57.73	430.2	73.1

