Appendix A.II

The Molar Heat Capacities of Gases in the Ideal Gas (Zero-Pressure) State*

		a	$b \times 10^2$	$c \times 10^5$	$d \times 10^9$	Temperature Range (K)
Paraffinic Hydrocarbons						
Methane	CH_4	19.875	5.021	1.268	−11.004	273–1500
Ethane	C_2H_6	6.895	17.255	−6.402	7.280	273–1500
Propane	C_3H_8	−4.042	30.456	−15.711	31.716	273–1500
n-Butane	C_4H_{10}	3.954	37.126	−18.326	34.979	273–1500
i-Butane	C_4H_{10}	−7.908	41.573	−22.992	49.875	273–1500
n-Pentane	C_5H_{12}	6.770	45.398	−22.448	42.259	273–1500
n-Hexane	C_6H_{14}	6.933	55.188	−28.636	57.657	273–1500
Monoolefinic Hydrocarbons						
Ethylene	C_2H_4	3.950	15.628	−8.339	17.657	273–1500
Propylene	C_3H_6	3.151	23.812	−12.176	24.603	273–1500
1-Butene	C_4H_8	−1.004	36.193	−21.381	50.502	273–1500
i-Butene	C_4H_8	6.904	32.226	−16.657	33.557	273–1500
cis-2-Butene	C_4H_8	−7.439	33.799	−17.046	33.013	273–1500
trans-2-Butene	C_4H_8	9.791	30.209	−14.239	25.398	273–1500
Cycloparaffinic Hydrocarbons						
Cyclopentane	C_5H_{10}	−54.213	54.757	−31.159	68.661	273–1500
Methylcyclopentane	C_6H_{12}	−50.686	64.352	−37.301	83.808	273–1500
Cyclohexane	C_6H_{12}	−66.674	68.845	−38.506	80.628	273–1500
Methylcyclohexane	C_7H_{14}	−63.054	79.381	−45.979	100.795	273–1500
Aromatic Hydrocarbons						
Benzene	C_6H_6	−36.193	48.444	−31.548	77.573	273–1500
Toluene	C_7H_8	−34.364	55.887	−34.435	80.335	273–1500
Ethylbenzene	C_8H_{10}	−35.138	66.674	−41.854	100.209	273–1500
Styrene	C_8H_8	−24.971	60.059	−38.285	92.176	273–1500
Cumene	C_9H_{12}	−39.548	78.184	−49.661	120.502	273–1500
Oxygenated Hydrocarbons						
Formaldehyde	CH_2O	22.791	4.075	0.713	−8.695	273–1500
Acetaldehyde	C_2H_4O	17.531	13.239	−2.155	−15.900	273–1000
Methanol	CH_4O	19.038	9.146	−1.218	−8.034	273–1000
Ethanol	C_2H_6O	19.875	20.946	−10.372	20.042	273–1500
Ethylene oxide	C_2H_4O	−4.686	20.607	−9.996	13.176	273–1000
Ketene	C_2H_2O	17.197	12.410	−7.502	17.657	273–1500

*Constants are for the equation $C_P^* = a + bT + cT^2 + dT^3$, where T is in kelvins and C_P^* in J (mol K)$^{-1}$.

Appendix II (*Continued*)

		a	$b \times 10^2$	$c \times 10^5$	$d \times 10^9$	Temperature Range (K)
Miscellaneous Hydrocarbons						
Cyclopropane	C_3H_6	−27.117	34.335	−23.335	65.314	273–1000
Isopentane	C_5H_{12}	−9.511	52.025	−29.695	66.360	273–1500
Neopentane	C_5H_{12}	16.172	55.670	−33.548	78.787	273–1500
o-Xylene	C_8H_{10}	−15.854	59.795	−34.954	78.661	273–1500
m-Xylene	C_8H_{10}	−27.335	62.364	−36.950	83.891	273–1500
p-Xylene	C_8H_{10}	−22.318	59.498	−33.406	71.255	273–1500
C_3 Oxygenated Hydrocarbons						
Carbon suboxide	C_3O_2	34.322	12.858	−8.707	21.682	273–1500
Acetone	C_3H_6O	6.799	27.870	−15.636	34.757	273–1500
i-Propyl alcohol	C_3H_8O	3.321	35.573	−20.987	48.368	273–1500
n-Propyl alcohol	C_3H_8O	−5.469	38.640	−24.268	59.163	273–1500
Allyl alcohol	C_3H_6O	2.177	29.799	−17.820	41.623	273–1500
Chloroethenes						
Chloroethene	C_2H_3Cl	10.046	17.866	−11.511	28.439	273–1500
1,1-Dichloroethene	$C_2H_2Cl_2$	24.682	18.339	−13.314	35.632	273–1500
cis-1,2-Dichloroethene	$C_2H_2Cl_2$	18.142	19.628	−14.213	37.699	273–1500
trans-1,2-Dichloroethene	$C_2H_2Cl_2$	23.686	17.971	−12.644	33.017	273–1500
Trichloroethene	C_2HCl_3	38.494	18.900	−15.063	42.259	273–1500
Tetrachloroethene	C_2Cl_4	63.222	15.895	−13.301	38.029	273–1500
Nitrogen Compounds						
Ammonia	NH_3	27.551	2.563	0.990	−6.687	273–1500
Hydrazine	N_2H_4	16.276	14.870	−9.640	25.063	273–1500
Methylamine	CH_5N	12.534	15.105	−6.881	12.345	273–1500
Dimethylamine	C_2H_7N	−1.151	27.679	−14.572	29.921	273–1500
Trimethylamine	C_3H_9N	−8.778	40.246	−23.217	52.017	273–1500
Halogens and Halogen Acids						
Fluorine	F_2	25.586	2.454	−1.752	4.099	273–2000
Chlorine	Cl_2	28.541	2.389	−2.137	6.473	273–1500
Bromine	Br_2	33.686	1.030	−0.890	2.680	273–1500
Iodine	I_2	35.582	0.550	−0.447	1.308	273–1800
Hydrogen fluoride	HF	30.130	−0.493	0.659	−1.573	273–2000
Hydrogen chloride	HCl	30.310	−0.762	1.326	−4.335	273–1500
Hydrogen bromide	HBr	29.996	−0.671	1.387	−4.858	273–1500
Hydrogen iodide	HI	28.042	0.190	0.509	−2.014	273–1900
Chloromethanes						
Methyl chloride	CH_3Cl	12.762	10.862	−5.205	9.623	273–1500
Methylene chloride	CH_2Cl_2	17.573	14.305	−9.833	25.389	273–1500
Chloroform	$CHCl_3$	31.841	14.481	−11.163	30.728	273–1500
Carbon tetrachloride	CCl_4	51.213	14.226	−12.531	36.937	273–1500
Phosgene	$COCl_2$	43.305	6.916	−3.518		273–1000
Thiophosgene	$CSCl_2$	45.188	7.778	−4.372		273–1000

Appendix II (*Continued*)

		a	$b \times 10^2$	$c \times 10^5$	$d \times 10^9$	Temperature Range (K)
Cyanogens						
Cyanogen	$(CN)_2$	41.088	6.217	−2.749		273–1000
Hydrogen cyanide	HCN	26.527	3.504	−1.093		273–1500
Cyanogen chloride	CNCl	33.347	4.496	−2.203		273–1000
Cyanogen bromide	CNBr	36.904	3.801	−1.827		273–1000
Cyanogen iodide	CNI	40.544	3.018	−1.366		273–1000
Acetonitrile	CH_3CN	21.297	11.562	−3.812		273–1200
Acrylic nitrile	CH_2CHCl	19.038	17.171	−7.087		273–1000
Oxides of Nitrogen						
Nitric oxide	NO	27.034	0.987	−0.322	0.365	273–3800
Nitric oxide	NO	29.322	−0.094	0.974	−4.184	273–1500
Nitrous oxide	N_2O	24.092	5.859	−3.560	10.569	273–1500
Nitrogen dioxide	NO_2	22.929	5.711	−3.519	7.866	273–1500
Nitrogen tetroxide	N_2O_4	33.054	18.661	−11.339		273–600
Acetylenes and Diolefins						
Acetylene	C_2H_2	21.799	9.208	−6.523	18.197	273–1500
Methylacetylene	C_3H_4	17.615	17.042	−9.172	19.720	273–1500
Dimethylacetylene	C_4H_6	14.812	24.427	−11.548	20.812	273–1500
Propadiene	C_3H_4	10.167	19.636	−11.636	27.130	273–1500
1,3-Butadiene	C_4H_6	−5.398	34.937	−23.356	59.582	273–1500
Isoprene	C_5H_8	−1.841	43.590	−28.293	70.837	273–1500
Combustion Gases (Low Range)						
Nitrogen	N_2	28.883	−0.157	0.808	−2.871	273–1800
Oxygen	O_2	25.460	1.519	−0.715	1.311	273–1800
Air		28.088	0.197	0.480	−1.965	273–1800
Hydrogen	H_2	29.088	−0.192	0.400	−0.870	273–1800
Carbon monoxide	CO	28.142	0.167	0.537	−2.221	273–1800
Carbon dioxide	CO_2	22.243	5.977	−3.499	7.464	273–1800
Water vapor	H_2O	32.218	0.192	1.055	−3.593	273–1800
Ammonia	NH_3	24.619	3.75	−0.138		300–1500
Combustion Gases (High Range)†						
Nitrogen	N_2	27.318	0.623	−0.095		273-3800
Oxygen	O_2	28.167	0.630	−0.075		273–3800
Air		27.435	0.618	−0.090		273–3800
Hydrogen	H_2	26.879	0.435	−0.033		273–3800
Carbon monoxide	CO	27.113	0.655	−0.100		273–3800
Water vapor	H_2O	29.163	1.449	−0.202		273–3800
Sulfur Compounds						
Sulfur	S_2	27.193	2.217	−1.627	3.983	273–1800
Sulfur dioxide	SO_2	25.762	5.791	−3.809	8.607	273–1800
Sulfur trioxide	SO_3	16.393	14.573	−11.193	32.402	273–1300
Hydrogen sulfide	H_2S	29.582	1.309	0.571	−3.292	273–1800
Carbon disulfide	CS_2	30.921	6.230	−4.586	11.548	273–1800
Carbonyl sulfide	COS	26.034	6.427	−4.427	10.711	273–1800

†The equation for CO_2 in the temperature range of 273–3800 K is $C_P^* = 75.464 - 1.872 \times 10^{-4}T - 661.42/\sqrt{T}$.

Based on data in O. Hougen, K. Watson, and R. A. Ragatz, *Chemical Process Principles,* Part 1, John Wiley & Sons, New York (1954). Used with permission.

Table 6.6-1 The Critical and Other Constants for Selected Fluids

Substance	Symbol	Molecular Weight (g mol^{-1})	T_c(K)	P_c(MPa)	V_c(m^3/kmol)	Z_c	ω	T_{boil}(K)
Acetylene	C_2H_2	26.038	308.3	6.140	0.113	0.271	0.184	189.2
Ammonia	NH_3	17.031	405.6	11.28	0.0724	0.242	0.250	239.7
Argon	Ar	39.948	150.8	4.874	0.0749	0.291	−0.004	87.3
Benzene	C_6H_6	78.114	562.1	4.894	0.259	0.271	0.212	353.3
n-Butane	C_4H_{10}	58.124	425.2	3.800	0.255	0.274	0.193	272.7
Isobutane	C_4H_{10}	58.124	408.1	3.648	0.263	0.283	0.176	261.3
1-Butene	C_4H_8	56.108	419.6	4.023	0.240	0.277	0.187	266.9
Carbon dioxide	CO_2	44.010	304.2	7.376	0.0940	0.274	0.225	194.7
Carbon monoxide	CO	28.010	132.9	3.496	0.0931	0.295	0.049	81.7
Carbon tetrachloride	CCl_4	153.823	556.4	4.560	0.276	0.272	0.194	349.7
n-Decane	$C_{10}H_{22}$	142.286	617.6	2.108	0.603	0.247	0.490	447.3
n-Dodecane	$C_{12}H_{26}$	170.340	658.3	1.824	0.713	0.24	0.562	489.5
Ethane	C_2H_6	30.070	305.4	4.884	0.148	0.285	0.098	184.5
Ethyl ether	$C_4H_{10}O$	74.123	466.7	3.638	0.280	0.262	0.281	307.7
Ethylene	C_2H_4	28.054	282.4	5.036	0.129	0.276	0.085	169.4
Helium	He	4.003	5.19	0.227	0.0573	0.301	−0.387	4.21
n-Heptane	C_7H_{16}	100.205	540.2	2.736	0.304	0.263	0.351	371.6
n-Hexane	C_6H_{14}	86.178	507.4	2.969	0.370	0.260	0.296	341.9
Hydrogen	H_2	2.016	33.2	1.297	0.065	0.305	−0.22	20.4
Hydrogen fluoride	HF	20.006	461.0	6.488	0.069	0.12	0.372	292.7
Hydrogen sulfide	H_2S	34.080	373.2	8.942	0.0985	0.284	0.100	212.8
Methane	CH_4	16.043	190.6	4.600	0.099	0.288	0.008	111.7
Naphthalene	$C_{10}H_8$	128.174	748.4	4.05	0.410	0.267	0.302	491.1
Neon	Ne	20.183	44.4	2.756	0.0417	0.311	0	27.0
Nitric oxide	NO	30.006	180.0	6.485	0.058	0.250	0.607	121.4
Nitrogen	N_2	28.013	126.2	3.394	0.0895	0.290	0.040	77.4
n-Octane	C_8H_{18}	114.232	568.8	2.482	0.492	0.259	0.394	398.8
Oxygen	O_2	31.999	154.6	5.046	0.0732	0.288	0.021	90.2
n-Pentane	C_5H_{12}	72.151	469.6	3.374	0.304	0.262	0.251	309.2
Isopentane	C_5H_{12}	72.151	460.4	3.384	0.306	0.271	0.227	301.0
Propane	C_3H_8	44.097	369.8	4.246	0.203	0.281	0.152	231.1
Propylene	C_3H_6	42.081	365.0	4.620	0.181	0.275	0.148	225.4
Refrigerant R12	CCl_2F_2	120.914	385.0	4.124	0.217	0.280	0.176	243.4
Refrigerant HFC-134a	CH_2FCF_3	102.03	374.23	4.060	0.198	0.258	0.332	247.1
Sulfur dioxide	SO_2	64.063	430.8	7.883	0.122	0.268	0.251	263
Toluene	C_7H_8	92.141	591.7	4.113	0.316	0.264	0.257	383.8
Water	H_2O	18.015	647.3	22.048	0.056	0.229	0.344	373.2
Xenon	Xe	131.300	289.7	5.836	0.118	0.286	0.002	165.0

Source: Adapted from R. C. Reid, J. M. Prausnitz, and B. E. Poling, *The Properties of Gases and Liquids,* 4th ed., McGraw-Hill, New York, 1986, Appendix A and other sources.

ior. (It is, however, a great improvement over the ideal gas equation of state, which predicts that $Z = 1$ for all conditions.)

The fact that the critical compressibility of the van der Waals fluid is not equal to that for most real fluids also means that different values for the van der Waals parameters are obtained for any one fluid, depending on whether Eqs. 6.6-3a, Eqs. 6.6-4a, or Eqs. 6.6-4b are used to relate these parameters to the critical properties. In practice, the