

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)
<i>Paraffinic Hydrocarbons</i>						
Methane	CH ₄	19.875	5.021	1.268	-11.004	273-1500
Ethane	C ₂ H ₆	6.895	17.255	-6.402	7.280	273-1500
Propane	C ₃ H ₈	-4.042	30.456	-15.711	31.716	273-1500
<i>n</i> -Butane	C ₄ H ₁₀	3.954	37.126	-18.326	34.979	273-1500
<i>i</i> -Butane	C ₄ H ₁₀	-7.908	41.573	-22.992	49.875	273-1500
<i>n</i> -Pentane	C ₅ H ₁₂	6.770	45.398	-22.448	42.259	273-1500
<i>n</i> -Hexane	C ₆ H ₁₄	6.933	55.188	-28.636	57.657	273-1500
<i>Monoolefinic Hydrocarbons</i>						
Ethylene	C ₂ H ₄	3.950	15.628	-8.339	17.657	273-1500
Propylene	C ₃ H ₆	3.151	23.812	-12.176	24.603	273-1500
1-Butene	C ₄ H ₈	-1.004	36.193	-21.381	50.502	273-1500
<i>i</i> -Butene	C ₄ H ₈	6.904	32.226	-16.657	33.557	273-1500
<i>cis</i> -2-Butene	C ₄ H ₈	-7.439	33.799	-17.046	33.013	273-1500
<i>trans</i> -2-Butene	C ₄ H ₈	9.791	30.209	-14.239	25.398	273-1500
<i>Cycloparaffinic Hydrocarbons</i>						
Cyclopentane	C ₅ H ₁₀	-54.213	54.757	-31.159	68.661	273-1500
Methylcyclopentane	C ₆ H ₁₂	-50.686	64.352	-37.301	83.808	273-1500
Cyclohexane	C ₆ H ₁₂	-66.674	68.845	-38.506	80.628	273-1500
Methylcyclohexane	C ₇ H ₁₄	-63.054	79.381	-45.979	100.795	273-1500
<i>Aromatic Hydrocarbons</i>						
Benzene	C ₆ H ₆	-36.193	48.444	-31.548	77.573	273-1500
Toluene	C ₇ H ₈	-34.364	55.887	-34.435	80.335	273-1500
Ethylbenzene	C ₈ H ₁₀	-35.138	66.674	-41.854	100.209	273-1500
Styrene	C ₈ H ₈	-24.971	60.059	-38.285	92.176	273-1500
Cumene	C ₉ H ₁₂	-39.548	78.184	-49.661	120.502	273-1500
<i>Oxygenated Hydrocarbons</i>						
Formaldehyde	CH ₂ O	22.791	4.075	0.713	-8.695	273-1500
Acetaldehyde	C ₂ H ₄ O	17.531	13.239	-2.155	-15.900	273-1000
Methanol	CH ₄ O	19.038	9.146	-1.218	-8.034	273-1000
Ethanol	C ₂ H ₆ O	19.875	20.946	-10.372	20.042	273-1500
Ethylene oxide	C ₂ H ₄ O	-4.686	20.607	-9.996	13.176	273-1000
Ketene	C ₂ H ₂ O	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 $\text{J}(\text{mol K})^{-1}$.

Appendix II (Continued)

		<i>a</i>	<i>b</i> × 10 ²	<i>c</i> × 10 ⁵	<i>d</i> × 10 ⁹	Temperature Range (K)
<i>Miscellaneous Hydrocarbons</i>						
Cyclopropane	C ₃ H ₆	-27.117	34.335	-23.335	65.314	273-1000
Isopentane	C ₅ H ₁₂	-9.511	52.025	-29.695	66.360	273-1500
Neopentane	C ₅ H ₁₂	16.172	55.670	-33.548	78.787	273-1500
<i>o</i> -Xylene	C ₈ H ₁₀	-15.854	59.795	-34.954	78.661	273-1500
<i>m</i> -Xylene	C ₈ H ₁₀	-27.335	62.364	-36.950	83.891	273-1500
<i>p</i> -Xylene	C ₈ H ₁₀	-22.318	59.498	-33.406	71.255	273-1500
<i>C₃ Oxygenated Hydrocarbons</i>						
Carbon suboxide	C ₃ O ₂	34.322	12.858	-8.707	21.682	273-1500
Acetone	C ₃ H ₆ O	6.799	27.870	-15.636	34.757	273-1500
<i>i</i> -Propyl alcohol	C ₃ H ₈ O	3.321	35.573	-20.987	48.368	273-1500
<i>n</i> -Propyl alcohol	C ₃ H ₈ O	-5.469	38.640	-24.268	59.163	273-1500
Allyl alcohol	C ₃ H ₆ O	2.177	29.799	-17.820	41.623	273-1500
<i>Chloroethenes</i>						
Chloroethene	C ₂ H ₃ Cl	10.046	17.866	-11.511	28.439	273-1500
1,1-Dichloroethene	C ₂ H ₂ Cl ₂	24.682	18.339	-13.314	35.632	273-1500
<i>cis</i> -1,2-Dichloroethene	C ₂ H ₂ Cl ₂	18.142	19.628	-14.213	37.699	273-1500
<i>trans</i> -1,2-Dichloroethene	C ₂ H ₂ Cl ₂	23.686	17.971	-12.644	33.017	273-1500
Trichloroethene	C ₂ HCl ₃	38.494	18.900	-15.063	42.259	273-1500
Tetrachloroethene	C ₂ Cl ₄	63.222	15.895	-13.301	38.029	273-1500
<i>Nitrogen Compounds</i>						
Ammonia	NH ₃	27.551	2.563	0.990	-6.687	273-1500
Hydrazine	N ₂ H ₄	16.276	14.870	-9.640	25.063	273-1500
Methylamine	CH ₅ N	12.534	15.105	-6.881	12.345	273-1500
Dimethylamine	C ₂ H ₇ N	-1.151	27.679	-14.572	29.921	273-1500
Trimethylamine	C ₃ H ₉ N	-8.778	40.246	-23.217	52.017	273-1500
<i>Halogens and Halogen Acids</i>						
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
<i>Chloromethanes</i>						
Methyl chloride	CH ₃ Cl	12.762	10.862	-5.205	9.623	273-1500
Methylene chloride	CH ₂ Cl 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)

		<i>a</i>	<i>b</i> × 10 ²	<i>c</i> × 10 ⁵	<i>d</i> × 10 ⁹	Temperature Range (K)
<i>Cyanogens</i>						
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 ₃ CN	21.297	11.562	-3.812		273-1200
Acrylic nitrile	CH ₂ CHCl	19.038	17.171	-7.087		273-1000
<i>Oxides of Nitrogen</i>						
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 ₂ O	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 ₂ O ₄	33.054	18.661	-11.339		273-600
<i>Acetylenes and Diolefins</i>						
Acetylene	C ₂ H ₂	21.799	9.208	-6.523	18.197	273-1500
Methylacetylene	C ₃ H ₄	17.615	17.042	-9.172	19.720	273-1500
Dimethylacetylene	C ₄ H ₆	14.812	24.427	-11.548	20.812	273-1500
Propadiene	C ₃ H ₄	10.167	19.636	-11.636	27.130	273-1500
1,3-Butadiene	C ₄ H ₆	-5.398	34.937	-23.356	59.582	273-1500
Isoprene	C ₅ H ₈	-1.841	43.590	-28.293	70.837	273-1500
<i>Combustion Gases (Low Range)</i>						
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 ₂ O	32.218	0.192	1.055	-3.593	273-1800
Ammonia	NH ₃	24.619	3.75	-0.138		300-1500
<i>Combustion Gases (High Range)†</i>						
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 ₂ O	29.163	1.449	-0.202		273-3800
<i>Sulfur Compounds</i>						
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 ₂ S	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 CO₂ 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).
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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 ₂ H 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 ₆ H ₆	78.114	562.1	4.894	0.259	0.271	0.212	353.3
<i>n</i> -Butane	C ₄ H ₁₀	58.124	425.2	3.800	0.255	0.274	0.193	272.7
Isobutane	C ₄ H ₁₀	58.124	408.1	3.648	0.263	0.283	0.176	261.3
1-Butene	C ₄ H 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
<i>n</i> -Decane	C ₁₀ H ₂₂	142.286	617.6	2.108	0.603	0.247	0.490	447.3
<i>n</i> -Dodecane	C ₁₂ H ₂₆	170.340	658.3	1.824	0.713	0.24	0.562	489.5
Ethane	C ₂ H ₆	30.070	305.4	4.884	0.148	0.285	0.098	184.5
Ethyl ether	C ₄ H ₁₀ O	74.123	466.7	3.638	0.280	0.262	0.281	307.7
Ethylene	C ₂ H 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
<i>n</i> -Heptane	C ₇ H ₁₆	100.205	540.2	2.736	0.304	0.263	0.351	371.6
<i>n</i> -Hexane	C ₆ H 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 ₂ S	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
<i>n</i> -Octane	C ₈ H 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
<i>n</i> -Pentane	C ₅ H ₁₂	72.151	469.6	3.374	0.304	0.262	0.251	309.2
Isopentane	C ₅ H ₁₂	72.151	460.4	3.384	0.306	0.271	0.227	301.0
Propane	C ₃ H ₈	44.097	369.8	4.246	0.203	0.281	0.152	231.1
Propylene	C ₃ H ₆	42.081	365.0	4.620	0.181	0.275	0.148	225.4
Refrigerant R12	CCl ₂ F ₂	120.914	385.0	4.124	0.217	0.280	0.176	243.4
Refrigerant HFC-134a	CH ₂ FCF 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 ₇ H ₈	92.141	591.7	4.113	0.316	0.264	0.257	383.8
Water	H ₂ O	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