

Appendix

A

Selected Thermodynamic Properties of Gases Comprising C–H–O–N System

TABLES A.1 TO A.12

Ideal-gas values for standard reference state ($T = 298.15$ K, $P = 1$ atm) for

$$\bar{c}_p(T), \bar{h}^o(T) - \bar{h}_{f, \text{ref}}^o, \bar{h}_f^o(T), \bar{s}^o(T), \bar{g}_f^o(T) \quad \text{for} \\ \text{CO, CO}_2, \text{H}_2, \text{H, OH, H}_2\text{O, N}_2, \text{N, NO, NO}_2, \text{O}_2, \text{O.}$$

Enthalpy of formation and Gibbs function of formation for compounds are calculated from the elements as

$$\begin{aligned} \bar{h}_{f,i}^o(T) &= \bar{h}_i^o(T) - \sum_{j \text{ elements}} \nu_j' \bar{h}_j^o(T) \\ \bar{g}_{f,i}^o(T) &= \bar{g}_i^o(T) - \sum_{j \text{ elements}} \nu_j' \bar{g}_j^o(T) \\ &= \bar{h}_{f,i}^o(T) - T \bar{s}_i^o(T) - \sum_{j \text{ elements}} \nu_j' [-T \bar{s}_j^o(T)] \end{aligned}$$

SOURCE: Tables were generated from curvefit coefficients given in Kee, R. J., Rupley, F. M., and Miller, J. A., "The Chemkin Thermodynamic Data Base," Sandia Report, SAND87-8215B, March 1991.

TABLE A.13

Curvefit coefficients for $\bar{c}_p(T)$ for the same gases as above.

SOURCE: *ibid.*

Table A.1 Carbon monoxide (CO), MW = 28.010, enthalpy of formation @ 298 K (kJ/kmol) = -110,541

$T(\text{K})$	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	28.687	-2,835	-111,308	186.018	-128,532
298	29.072	0	-110,541	197.548	-137,163
300	29.078	54	-110,530	197.728	-137,328
400	29.433	2,979	-110,121	206.141	-146,332
500	29.857	5,943	-110,017	212.752	-155,403
600	30.407	8,955	-110,156	218.242	-164,470
700	31.089	12,029	-110,477	222.979	-173,499
800	31.860	15,176	-110,924	227.180	-182,473
900	32.629	18,401	-111,450	230.978	-191,386
1000	33.255	21,697	-112,022	234.450	-200,238
1100	33.725	25,046	-112,619	237.642	-209,030
1200	34.148	28,440	-113,240	240.595	-217,768
1300	34.530	31,874	-113,881	243.344	-226,453
1400	34.872	35,345	-114,543	245.915	-235,087
1500	35.178	38,847	-115,225	248.332	-243,674
1600	35.451	42,379	-115,925	250.611	-252,214
1700	35.694	45,937	-116,644	252.768	-260,711
1800	35.910	49,517	-117,380	254.814	-269,164
1900	36.101	53,118	-118,132	256.761	-277,576
2000	36.271	56,737	-118,902	258.617	-285,948
2100	36.421	60,371	-119,687	260.391	-294,281
2200	36.553	64,020	-120,488	262.088	-302,576
2300	36.670	67,682	-121,305	263.715	-310,835
2400	36.774	71,354	-122,137	265.278	-319,057
2500	36.867	75,036	-122,984	266.781	-327,245
2600	36.950	78,727	-123,847	268.229	-335,399
2700	37.025	82,426	-124,724	269.625	-343,519
2800	37.093	86,132	-125,616	270.973	-351,606
2900	37.155	89,844	-126,523	272.275	-359,661
3000	37.213	93,562	-127,446	273.536	-367,684
3100	37.268	97,287	-128,383	274.757	-375,677
3200	37.321	101,016	-129,335	275.941	-383,639
3300	37.372	104,751	-130,303	277.090	-391,571
3400	37.422	108,490	-131,285	278.207	-399,474
3500	37.471	112,235	-132,283	279.292	-407,347
3600	37.521	115,985	-133,295	280.349	-415,192
3700	37.570	119,739	-134,323	281.377	-423,008
3800	37.619	123,499	-135,366	282.380	-430,796
3900	37.667	127,263	-136,424	283.358	-438,557
4000	37.716	131,032	-137,497	284.312	-446,291
4100	37.764	134,806	-138,585	285.244	-453,997
4200	37.810	138,585	-139,687	286.154	-461,677
4300	37.855	142,368	-140,804	287.045	-469,330
4400	37.897	146,156	-141,935	287.915	-476,957
4500	37.936	149,948	-143,079	288.768	-484,558
4600	37.970	153,743	-144,236	289.602	-492,134
4700	37.998	157,541	-145,407	290.419	-499,684
4800	38.019	161,342	-146,589	291.219	-507,210
4900	38.031	165,145	-147,783	292.003	-514,710
5000	38.033	168,948	-148,987	292.771	-522,186

Table A.2 Carbon dioxide (CO₂), MW = 44.011, enthalpy of formation @ 298 K (kJ/kmol) = -393,546

$T(K)$	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	32.387	-3,423	-393,483	199.876	-394,126
298	37.198	0	-393,546	213.736	-394,428
300	37.280	69	-393,547	213.966	-394,433
400	41.276	4,003	-393,617	225.257	-394,718
500	44.569	8,301	-393,712	234.833	-394,983
600	47.313	12,899	-393,844	243.209	-395,226
700	49.617	17,749	-394,013	250.680	-395,443
800	51.550	22,810	-394,213	257.436	-395,635
900	53.136	28,047	-394,433	263.603	-395,799
1000	54.360	33,425	-394,659	269.268	-395,939
1100	55.333	38,911	-394,875	274.495	-396,056
1200	56.205	44,488	-395,083	279.348	-396,155
1300	56.984	50,149	-395,287	283.878	-396,236
1400	57.677	55,882	-395,488	288.127	-396,301
1500	58.292	61,681	-395,691	292.128	-396,352
1600	58.836	67,538	-395,897	295.908	-396,389
1700	59.316	73,446	-396,110	299.489	-396,414
1800	59.738	79,399	-396,332	302.892	-396,425
1900	60.108	85,392	-396,564	306.132	-396,424
2000	60.433	91,420	-396,808	309.223	-396,410
2100	60.717	97,477	-397,065	312.179	-396,384
2200	60.966	103,562	-397,338	315.009	-396,346
2300	61.185	109,670	-397,626	317.724	-396,294
2400	61.378	115,798	-397,931	320.333	-396,230
2500	61.548	121,944	-398,253	322.842	-396,152
2600	61.701	128,107	-398,594	325.259	-396,061
2700	61.839	134,284	-398,952	327.590	-395,957
2800	61.965	140,474	-399,329	329.841	-395,840
2900	62.083	146,677	-399,725	332.018	-395,708
3000	62.194	152,891	-400,140	334.124	-395,562
3100	62.301	159,116	-400,573	336.165	-395,403
3200	62.406	165,351	-401,025	338.145	-395,229
3300	62.510	171,597	-401,495	340.067	-395,041
3400	62.614	177,853	-401,983	341.935	-394,838
3500	62.718	184,120	-402,489	343.751	-394,620
3600	62.825	190,397	-403,013	345.519	-394,388
3700	62.932	196,685	-403,553	347.242	-394,141
3800	63.041	202,983	-404,110	348.922	-393,879
3900	63.151	209,293	-404,684	350.561	-393,602
4000	63.261	215,613	-405,273	353.161	-393,311
4100	63.369	221,945	-405,878	353.725	-393,004
4200	63.474	228,287	-406,499	355.253	-392,683
4300	63.575	234,640	-407,135	356.748	-392,346
4400	63.669	241,002	-407,785	358.210	-391,995
4500	63.753	247,373	-408,451	359.642	-391,629
4600	63.825	253,752	-409,132	361.044	-391,247
4700	63.881	260,138	-409,828	362.417	-390,851
4800	63.918	266,528	-410,539	363.763	-390,440
4900	63.932	272,920	-411,267	365.081	-390,014
5000	63.919	279,313	-412,010	366.372	-389,572

Table A.3 Hydrogen (H₂), MW = 2.016, enthalpy of formation @ 298 K (kJ/kmol) = 0

$T(\text{K})$	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	28.522	-2,818	0	119.137	0
298	28.871	0	0	130.595	0
300	28.877	53	0	130.773	0
400	29.120	2,954	0	139.116	0
500	29.275	5,874	0	145.632	0
600	29.375	8,807	0	150.979	0
700	29.461	11,749	0	155.514	0
800	29.581	14,701	0	159.455	0
900	29.792	17,668	0	162.950	0
1000	30.160	20,664	0	166.106	0
1100	30.625	23,704	0	169.003	0
1200	31.077	26,789	0	171.687	0
1300	31.516	29,919	0	174.192	0
1400	31.943	33,092	0	176.543	0
1500	32.356	36,307	0	178.761	0
1600	32.758	39,562	0	180.862	0
1700	33.146	42,858	0	182.860	0
1800	33.522	46,191	0	184.765	0
1900	33.885	49,562	0	186.587	0
2000	34.236	52,968	0	188.334	0
2100	34.575	56,408	0	190.013	0
2200	34.901	59,882	0	191.629	0
2300	35.216	63,388	0	193.187	0
2400	35.519	66,925	0	194.692	0
2500	35.811	70,492	0	196.148	0
2600	36.091	74,087	0	197.558	0
2700	36.361	77,710	0	198.926	0
2800	36.621	81,359	0	200.253	0
2900	36.871	85,033	0	201.542	0
3000	37.112	88,733	0	202.796	0
3100	37.343	92,455	0	204.017	0
3200	37.566	96,201	0	205.206	0
3300	37.781	99,968	0	206.365	0
3400	37.989	103,757	0	207.496	0
3500	38.190	107,566	0	208.600	0
3600	38.385	111,395	0	209.679	0
3700	38.574	115,243	0	210.733	0
3800	38.759	119,109	0	211.764	0
3900	38.939	122,994	0	212.774	0
4000	39.116	126,897	0	213.762	0
4100	39.291	130,817	0	214.730	0
4200	39.464	134,755	0	215.679	0
4300	39.636	138,710	0	216.609	0
4400	39.808	142,682	0	217.522	0
4500	39.981	146,672	0	218.419	0
4600	40.156	150,679	0	219.300	0
4700	40.334	154,703	0	220.165	0
4800	40.516	158,746	0	221.016	0
4900	40.702	162,806	0	221.853	0
5000	40.895	166,886	0	222.678	0

Table A.4 Hydrogen atom (H), MW = 1.008, enthalpy of formation @ 298 K (kJ/kmol) = 217,977

T (K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	20.786	-2,040	217,346	106.305	207,999
298	20.786	0	217,977	114.605	203,276
300	20.786	38	217,989	114.733	203,185
400	20.786	2,117	218,617	120.713	198,155
500	20.786	4,196	219,236	125.351	192,968
600	20.786	6,274	219,848	129.351	187,657
700	20.786	8,353	220,456	132.345	182,244
800	20.786	10,431	221,059	135.121	176,744
900	20.786	12,510	221,653	137.569	171,169
1000	20.786	14,589	222,234	139.759	165,528
1100	20.786	16,667	222,793	141.740	159,830
1200	20.786	18,746	223,329	143.549	154,082
1300	20.786	20,824	223,843	145.213	148,291
1400	20.786	22,903	224,335	146.753	142,461
1500	20.786	24,982	224,806	148.187	136,596
1600	20.786	27,060	225,256	149.528	130,700
1700	20.786	29,139	225,687	150.789	124,777
1800	20.786	31,217	226,099	151.977	118,830
1900	20.786	33,296	226,493	153.101	112,859
2000	20.786	35,375	226,868	154.167	106,869
2100	20.786	37,453	227,226	155.181	100,860
2200	20.786	39,532	227,568	156.148	94,834
2300	20.786	41,610	227,894	157.072	88,794
2400	20.786	43,689	228,204	157.956	82,739
2500	20.786	45,768	228,499	158.805	76,672
2600	20.786	47,846	228,780	159.620	70,593
2700	20.786	49,925	229,047	160.405	64,504
2800	20.786	52,003	229,301	161.161	58,405
2900	20.786	54,082	229,543	161.890	52,298
3000	20.786	56,161	229,772	162.595	46,182
3100	20.786	58,239	229,989	163.276	40,058
3200	20.786	60,318	230,195	163.936	33,928
3300	20.786	62,396	230,390	164.576	27,792
3400	20.786	64,475	230,574	165.196	21,650
3500	20.786	66,554	230,748	165.799	15,502
3600	20.786	68,632	230,912	166.384	9,350
3700	20.786	70,711	231,067	166.954	3,194
3800	20.786	72,789	231,212	167.508	-2,967
3900	20.786	74,868	231,348	168.048	-9,132
4000	20.786	76,947	231,475	168.575	-15,299
4100	20.786	79,025	231,594	169.088	-21,470
4200	20.786	81,104	231,704	169.589	-27,644
4300	20.786	83,182	231,805	170.078	-33,820
4400	20.786	85,261	231,897	170.556	-39,998
4500	20.786	87,340	231,981	171.023	-46,179
4600	20.786	89,418	232,056	171.480	-52,361
4700	20.786	91,497	232,123	171.927	-58,545
4800	20.786	93,575	232,180	172.364	-64,730
4900	20.786	95,654	232,228	172.793	-70,916
5000	20.786	97,733	232,267	173.213	-77,103

Table A.5 Hydroxyl (OH), MW = 17.007, enthalpy of formation @ 298 K (kJ/kmol) = 38,985

T (K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	30.140	-2,948	38,864	171.607	35,808
298	29.932	0	38,985	183.604	34,279
300	29.928	55	38,987	183.789	34,250
400	29.718	3,037	39,030	192.369	32,662
500	29.570	6,001	39,000	198.983	31,072
600	29.527	8,955	38,909	204.369	29,494
700	29.615	11,911	38,770	208.925	27,935
800	29.844	14,883	38,599	212.893	26,399
900	30.208	17,884	38,410	216.428	24,885
1000	30.682	20,928	38,220	219.635	23,392
1100	31.186	24,022	38,039	222.583	21,918
1200	31.662	27,164	37,867	225.317	20,460
1300	32.114	30,353	37,704	227.869	19,017
1400	32.540	33,586	37,548	230.265	17,585
1500	32.943	36,860	37,397	232.524	16,164
1600	33.323	40,174	37,252	234.662	14,753
1700	33.682	43,524	37,109	236.693	13,352
1800	34.019	46,910	36,969	238.628	11,958
1900	34.337	50,328	36,831	240.476	10,573
2000	34.635	53,776	36,693	242.245	9,194
2100	34.915	57,254	36,555	243.942	7,823
2200	35.178	60,759	36,416	245.572	6,458
2300	35.425	64,289	36,276	247.141	5,099
2400	35.656	67,843	36,133	248.654	3,746
2500	35.872	71,420	35,986	250.114	2,400
2600	36.074	75,017	35,836	251.525	1,060
2700	36.263	78,634	35,682	252.890	-275
2800	36.439	82,269	35,524	254.212	-1,604
2900	36.604	85,922	35,360	255.493	-2,927
3000	36.759	89,590	35,191	256.737	-4,245
3100	36.903	93,273	35,016	257.945	-5,556
3200	37.039	96,970	34,835	259.118	-6,862
3300	37.166	100,681	34,648	260.260	-8,162
3400	37.285	104,403	34,454	261.371	-9,457
3500	37.398	108,137	34,253	262.454	-10,745
3600	37.504	111,882	34,046	263.509	-12,028
3700	37.605	115,638	33,831	264.538	-13,305
3800	37.701	119,403	33,610	265.542	-14,576
3900	37.793	123,178	33,381	266.522	-15,841
4000	37.882	126,962	33,146	267.480	-17,100
4100	37.968	130,754	32,903	268.417	-18,353
4200	38.052	134,555	32,654	269.333	-19,600
4300	38.135	138,365	32,397	270.229	-20,841
4400	38.217	142,182	32,134	271.107	-22,076
4500	38.300	146,008	31,864	271.967	-23,306
4600	38.382	149,842	31,588	272.809	-24,528
4700	38.466	153,685	31,305	273.636	-25,745
4800	38.552	157,536	31,017	274.446	-26,956
4900	38.640	161,395	30,722	275.242	-28,161
5000	38.732	165,264	30,422	276.024	-29,360

Table A.6 Water (H₂O), MW = 18.016, enthalpy of formation @ 298 K (kJ/kmol) = -241,845, enthalpy of vaporization (kJ/kmol) = 44,010

$T(K)$	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	32.255	-3,227	-240,838	175.602	-232,779
298	33.448	0	-241,845	188.715	-228,608
300	33.468	62	-241,865	188.922	-228,526
400	34.437	3,458	-242,858	198.686	-223,929
500	35.337	6,947	-243,822	206.467	-219,085
600	36.288	10,528	-244,753	212.992	-214,049
700	37.364	14,209	-245,638	218.665	-208,861
800	38.587	18,005	-246,461	223.733	-203,550
900	39.930	21,930	-247,209	228.354	-198,141
1000	41.315	25,993	-247,879	232.633	-192,652
1100	42.638	30,191	-248,475	236.634	-187,100
1200	43.874	34,518	-249,005	240.397	-181,497
1300	45.027	38,963	-249,477	243.955	-175,852
1400	46.102	43,520	-249,895	247.332	-170,172
1500	47.103	48,181	-250,267	250.547	-164,464
1600	48.035	52,939	-250,597	253.617	-158,733
1700	48.901	57,786	-250,890	256.556	-152,983
1800	49.705	62,717	-251,151	259.374	-147,216
1900	50.451	67,725	-251,384	262.081	-141,435
2000	51.143	72,805	-251,594	264.687	-135,643
2100	51.784	77,952	-251,783	267.198	-129,841
2200	52.378	83,160	-251,955	269.621	-124,030
2300	52.927	88,426	-252,113	271.961	-118,211
2400	53.435	93,744	-252,261	274.225	-112,386
2500	53.905	99,112	-252,399	276.416	-106,555
2600	54.340	104,524	-252,532	278.539	-100,719
2700	54.742	109,979	-252,659	280.597	-94,878
2800	55.115	115,472	-252,785	282.595	-89,031
2900	55.459	121,001	-252,909	284.535	-83,181
3000	55.779	126,563	-253,034	286.420	-77,326
3100	56.076	132,156	-253,161	288.254	-71,467
3200	56.353	137,777	-253,290	290.039	-65,604
3300	56.610	143,426	-253,423	291.777	-59,737
3400	56.851	149,099	-253,561	293.471	-53,865
3500	57.076	154,795	-253,704	295.122	-47,990
3600	57.288	160,514	-253,852	296.733	-42,110
3700	57.488	166,252	-254,007	298.305	-36,226
3800	57.676	172,011	-254,169	299.841	-30,338
3900	57.856	177,787	-254,338	301.341	-24,446
4000	58.026	183,582	-254,515	302.808	-18,549
4100	58.190	189,392	-254,699	304.243	-12,648
4200	58.346	195,219	-254,892	305.647	-6,742
4300	58.496	201,061	-255,093	307.022	-831
4400	58.641	206,918	-255,303	308.368	5,085
4500	58.781	212,790	-255,522	309.688	11,005
4600	58.916	218,674	-255,751	310.981	16,930
4700	59.047	224,573	-255,990	312.250	22,861
4800	59.173	230,484	-256,239	313.494	28,796
4900	59.295	236,407	-256,501	314.716	34,737
5000	59.412	242,343	-256,774	315.915	40,684

Table A.7 Nitrogen (N₂), MW = 28.013, enthalpy of formation @ 298 K (kJ/kmol) = 0

T (K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	28.793	-2,841	0	179.959	0
298	29.071	0	0	191.511	0
300	29.075	54	0	191.691	0
400	29.319	2,973	0	200.088	0
500	29.636	5,920	0	206.662	0
600	30.086	8,905	0	212.103	0
700	30.684	11,942	0	216.784	0
800	31.394	15,046	0	220.927	0
900	32.131	18,222	0	224.667	0
1000	32.762	21,468	0	228.087	0
1100	33.258	24,770	0	231.233	0
1200	33.707	28,118	0	234.146	0
1300	34.113	31,510	0	236.861	0
1400	34.477	34,939	0	239.402	0
1500	34.805	38,404	0	241.792	0
1600	35.099	41,899	0	244.048	0
1700	35.361	45,423	0	246.184	0
1800	35.595	48,971	0	248.212	0
1900	35.803	52,541	0	250.142	0
2000	35.988	56,130	0	251.983	0
2100	36.152	59,738	0	253.743	0
2200	36.298	63,360	0	255.429	0
2300	36.428	66,997	0	257.045	0
2400	36.543	70,645	0	258.598	0
2500	36.645	74,305	0	260.092	0
2600	36.737	77,974	0	261.531	0
2700	36.820	81,652	0	262.919	0
2800	36.895	85,338	0	264.259	0
2900	36.964	89,031	0	265.555	0
3000	37.028	92,730	0	266.810	0
3100	37.088	96,436	0	268.025	0
3200	37.144	100,148	0	269.203	0
3300	37.198	103,865	0	270.347	0
3400	37.251	107,587	0	271.458	0
3500	37.302	111,315	0	272.539	0
3600	37.352	115,048	0	273.590	0
3700	37.402	118,786	0	274.614	0
3800	37.452	122,528	0	275.612	0
3900	37.501	126,276	0	276.586	0
4000	37.549	130,028	0	277.536	0
4100	37.597	133,786	0	278.464	0
4200	37.643	137,548	0	279.370	0
4300	37.688	141,314	0	280.257	0
4400	37.730	145,085	0	281.123	0
4500	37.768	148,860	0	281.972	0
4600	37.803	152,639	0	282.802	0
4700	37.832	156,420	0	283.616	0
4800	37.854	160,205	0	284.412	0
4900	37.868	163,991	0	285.193	0
5000	37.873	167,778	0	285.958	0

Table A.8 Nitrogen atom (N), $MW = 14.007$, enthalpy of formation @ 298 K (kJ/kmol) = 472,629

T (K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	20.790	-2,040	472,008	144.889	461,026
298	20.786	0	472,629	153.189	455,504
300	20.786	38	472,640	153.317	455,398
400	20.786	2,117	473,258	159.297	449,557
500	20.786	4,196	473,864	163.935	443,562
600	20.786	6,274	474,450	167.725	437,446
700	20.786	8,353	475,010	170.929	431,234
800	20.786	10,431	475,537	173.705	424,944
900	20.786	12,510	476,027	176.153	418,590
1000	20.786	14,589	476,483	178.343	412,183
1100	20.792	16,668	476,911	180.325	405,732
1200	20.795	18,747	477,316	182.134	399,243
1300	20.795	20,826	477,700	183.798	392,721
1400	20.793	22,906	478,064	185.339	386,171
1500	20.790	24,985	478,411	186.774	379,595
1600	20.786	27,064	478,742	188.115	372,996
1700	20.782	29,142	479,059	189.375	366,377
1800	20.779	31,220	479,363	190.563	359,740
1900	20.777	33,298	479,656	191.687	353,086
2000	20.776	35,376	479,939	192.752	346,417
2100	20.778	37,453	480,213	193.766	339,735
2200	20.783	39,531	480,479	194.733	333,039
2300	20.791	41,610	480,740	195.657	326,331
2400	20.802	43,690	480,995	196.542	319,612
2500	20.818	45,771	481,246	197.391	312,883
2600	20.838	47,853	481,494	198.208	306,143
2700	20.864	49,938	481,740	198.995	299,394
2800	20.895	52,026	481,985	199.754	292,636
2900	20.931	54,118	482,230	200.488	285,870
3000	20.974	56,213	482,476	201.199	279,094
3100	21.024	58,313	482,723	201.887	272,311
3200	21.080	60,418	482,972	202.555	265,519
3300	21.143	62,529	483,224	203.205	258,720
3400	21.214	64,647	483,481	203.837	251,913
3500	21.292	66,772	483,742	204.453	245,099
3600	21.378	68,905	484,009	205.054	238,276
3700	21.472	71,048	484,283	205.641	231,447
3800	21.575	73,200	484,564	206.215	224,610
3900	21.686	75,363	484,853	206.777	217,765
4000	21.805	77,537	485,151	207.328	210,913
4100	21.934	79,724	485,459	207.868	204,053
4200	22.071	81,924	485,779	208.398	197,186
4300	22.217	84,139	486,110	208.919	190,310
4400	22.372	86,368	486,453	209.431	183,427
4500	22.536	88,613	486,811	209.936	176,536
4600	22.709	90,875	487,184	210.433	169,637
4700	22.891	93,155	487,573	210.923	162,730
4800	23.082	95,454	487,979	211.407	155,814
4900	23.282	97,772	488,405	211.885	148,890
5000	23.491	100,111	488,850	212.358	141,956

Table A.9 Nitric oxide (NO), MW = 30.006, enthalpy of formation @ 298 K (kJ/kmol) = 90,297

T (K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	29.374	-2,901	90,234	198.856	87,811
298	29.728	0	90,297	210.652	86,607
300	29.735	55	90,298	210.836	86,584
400	30.103	3,046	90,341	219.439	85,340
500	30.570	6,079	90,367	226.204	84,086
600	31.174	9,165	90,382	231.829	82,828
700	31.908	12,318	90,393	236.688	81,568
800	32.715	15,549	90,405	241.001	80,307
900	33.489	18,860	90,421	244.900	79,043
1000	34.076	22,241	90,443	248.462	77,778
1100	34.483	25,669	90,465	251.729	76,510
1200	34.850	29,136	90,486	254.745	75,241
1300	35.180	32,638	90,505	257.548	73,970
1400	35.474	36,171	90,520	260.166	72,697
1500	35.737	39,732	90,532	262.623	71,423
1600	35.972	43,317	90,538	264.937	70,149
1700	36.180	46,925	90,539	267.124	68,875
1800	36.364	50,552	90,534	269.197	67,601
1900	36.527	54,197	90,523	271.168	66,327
2000	36.671	57,857	90,505	273.045	65,054
2100	36.797	61,531	90,479	274.838	63,782
2200	36.909	65,216	90,447	276.552	62,511
2300	37.008	68,912	90,406	278.195	61,243
2400	37.095	72,617	90,358	279.772	59,976
2500	37.173	76,331	90,303	281.288	58,711
2600	37.242	80,052	90,239	282.747	57,448
2700	37.305	83,779	90,168	284.154	56,188
2800	37.362	87,513	90,089	285.512	54,931
2900	37.415	91,251	90,003	286.824	53,677
3000	37.464	94,995	89,909	288.093	52,426
3100	37.511	98,744	89,809	289.322	51,178
3200	37.556	102,498	89,701	290.514	49,934
3300	37.600	106,255	89,586	291.670	48,693
3400	37.643	110,018	89,465	292.793	47,456
3500	37.686	113,784	89,337	293.885	46,222
3600	37.729	117,555	89,203	294.947	44,992
3700	37.771	121,330	89,063	295.981	43,766
3800	37.815	125,109	88,918	296.989	42,543
3900	37.858	128,893	88,767	297.972	41,325
4000	37.900	132,680	88,611	298.931	40,110
4100	37.943	136,473	88,449	299.867	38,900
4200	37.984	140,269	88,283	300.782	37,693
4300	38.023	144,069	88,112	301.677	36,491
4400	38.060	147,873	87,936	302.551	35,292
4500	38.093	151,681	87,755	303.407	34,098
4600	38.122	155,492	87,569	304.244	32,908
4700	38.146	159,305	87,379	305.064	31,721
4800	38.162	163,121	87,184	305.868	30,539
4900	38.171	166,938	86,984	306.655	29,361
5000	38.170	170,755	86,779	307.426	28,187

Table A.10 Nitrogen dioxide (NO₂), MW = 46.006, enthalpy of formation @ 298 K (kJ/kmol) = 33, 098

T (K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	32.936	-3,432	33,961	226.016	45,453
298	36.881	0	33,098	239.925	51,291
300	36.949	68	33,085	240.153	51,403
400	40.331	3,937	32,521	251.259	57,602
500	43.227	8,118	32,173	260.578	63,916
600	45.737	12,569	31,974	268.686	70,285
700	47.913	17,255	31,885	275.904	76,679
800	49.762	22,141	31,880	282.427	83,079
900	51.243	27,195	31,938	288.377	89,476
1000	52.271	32,375	32,035	293.834	95,864
1100	52.989	37,638	32,146	298.850	102,242
1200	53.625	42,970	32,267	303.489	108,609
1300	54.186	48,361	32,392	307.804	114,966
1400	54.679	53,805	32,519	311.838	121,313
1500	55.109	59,295	32,643	315.625	127,651
1600	55.483	64,825	32,762	319.194	133,981
1700	55.805	70,390	32,873	322.568	140,303
1800	56.082	75,984	32,973	325.765	146,620
1900	56.318	81,605	33,061	328.804	152,931
2000	56.517	87,247	33,134	331.698	159,238
2100	56.685	92,907	33,192	334.460	165,542
2200	56.826	98,583	33,233	337.100	171,843
2300	56.943	104,271	33,256	339.629	178,143
2400	57.040	109,971	33,262	342.054	184,442
2500	57.121	115,679	33,248	344.384	190,742
2600	57.188	121,394	33,216	346.626	197,042
2700	57.244	127,116	33,165	348.785	203,344
2800	57.291	132,843	33,095	350.868	209,648
2900	57.333	138,574	33,007	352.879	215,955
3000	57.371	144,309	32,900	354.824	222,265
3100	57.406	150,048	32,776	356.705	228,579
3200	57.440	155,791	32,634	358.529	234,898
3300	57.474	161,536	32,476	360.297	241,221
3400	57.509	167,285	32,302	362.013	247,549
3500	57.546	173,038	32,113	363.680	253,883
3600	57.584	178,795	31,908	365.302	260,222
3700	57.624	184,555	31,689	366.880	266,567
3800	57.665	190,319	31,456	368.418	272,918
3900	57.708	196,088	31,210	369.916	279,276
4000	57.750	201,861	30,951	371.378	285,639
4100	57.792	207,638	30,678	372.804	292,010
4200	57.831	213,419	30,393	374.197	298,387
4300	57.866	219,204	30,095	375.559	304,772
4400	57.895	224,992	29,783	376.889	311,163
4500	57.915	230,783	29,457	378.190	317,562
4600	57.925	236,575	29,117	379.464	323,968
4700	57.922	242,367	28,761	380.709	330,381
4800	57.902	248,159	28,389	381.929	336,803
4900	57.862	253,947	27,998	383.122	343,232
5000	57.798	259,730	27,586	384.290	349,670

Table A.11 Oxygen (O₂), MW = 31.999, enthalpy of formation @ 298 K (kJ/kmol) = 0

T (K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	28.473	-2,836	0	193.518	0
298	29.315	0	0	205.043	0
300	29.331	54	0	205.224	0
400	30.210	3,031	0	213.782	0
500	31.114	6,097	0	220.620	0
600	32.030	9,254	0	226.374	0
700	32.927	12,503	0	231.379	0
800	33.757	15,838	0	235.831	0
900	34.454	19,250	0	239.849	0
1000	34.936	22,721	0	243.507	0
1100	35.270	26,232	0	246.852	0
1200	35.593	29,775	0	249.935	0
1300	35.903	33,350	0	252.796	0
1400	36.202	36,955	0	255.468	0
1500	36.490	40,590	0	257.976	0
1600	36.768	44,253	0	260.339	0
1700	37.036	47,943	0	262.577	0
1800	37.296	51,660	0	264.701	0
1900	37.546	55,402	0	266.724	0
2000	37.788	59,169	0	268.656	0
2100	38.023	62,959	0	270.506	0
2200	38.250	66,773	0	272.280	0
2300	38.470	70,609	0	273.985	0
2400	38.684	74,467	0	275.627	0
2500	38.891	78,346	0	277.210	0
2600	39.093	82,245	0	278.739	0
2700	39.289	86,164	0	280.218	0
2800	39.480	90,103	0	281.651	0
2900	39.665	94,060	0	283.039	0
3000	39.846	98,036	0	284.387	0
3100	40.023	102,029	0	285.697	0
3200	40.195	106,040	0	286.970	0
3300	40.362	110,068	0	288.209	0
3400	40.526	114,112	0	289.417	0
3500	40.686	118,173	0	290.594	0
3600	40.842	122,249	0	291.742	0
3700	40.994	126,341	0	292.863	0
3800	41.143	130,448	0	293.959	0
3900	41.287	134,570	0	295.029	0
4000	41.429	138,705	0	296.076	0
4100	41.566	142,855	0	297.101	0
4200	41.700	147,019	0	298.104	0
4300	41.830	151,195	0	299.087	0
4400	41.957	155,384	0	300.050	0
4500	42.079	159,586	0	300.994	0
4600	42.197	163,800	0	301.921	0
4700	42.312	168,026	0	302.829	0
4800	42.421	172,262	0	303.721	0
4900	42.527	176,510	0	304.597	0
5000	42.627	180,767	0	305.457	0

Table A.12 Oxygen atom (O), MW = 16.000, enthalpy of formation @ 298 K (kJ/kmol) = 249,197

T (K)	$\bar{c}_p$ (kJ/kmol-K)	$(\bar{h}^o(T) - \bar{h}_f^o(298))$ (kJ/kmol)	$\bar{h}_f^o(T)$ (kJ/kmol)	$\bar{s}^o(T)$ (kJ/kmol-K)	$\bar{g}_f^o(T)$ (kJ/kmol)
200	22.477	-2,176	248,439	152.085	237,374
298	21.899	0	249,197	160.945	231,778
300	21.890	41	249,211	161.080	231,670
400	21.500	2,209	249,890	167.320	225,719
500	21.256	4,345	250,494	172.089	219,605
600	21.113	6,463	251,033	175.951	213,375
700	21.033	8,570	251,516	179.199	207,060
800	20.986	10,671	251,949	182.004	200,679
900	20.952	12,768	252,340	184.474	194,246
1000	20.915	14,861	252,698	186.679	187,772
1100	20.898	16,952	253,033	188.672	181,263
1200	20.882	19,041	253,350	190.490	174,724
1300	20.867	21,128	253,650	192.160	168,159
1400	20.854	23,214	253,934	193.706	161,572
1500	20.843	25,299	254,201	195.145	154,966
1600	20.834	27,383	254,454	196.490	148,342
1700	20.827	29,466	254,692	197.753	141,702
1800	20.822	31,548	254,916	198.943	135,049
1900	20.820	33,630	255,127	200.069	128,384
2000	20.819	35,712	255,325	201.136	121,709
2100	20.821	37,794	255,512	202.152	115,023
2200	20.825	39,877	255,687	203.121	108,329
2300	20.831	41,959	255,852	204.047	101,627
2400	20.840	44,043	256,007	204.933	94,918
2500	20.851	46,127	256,152	205.784	88,203
2600	20.865	48,213	256,288	206.602	81,483
2700	20.881	50,300	256,416	207.390	74,757
2800	20.899	52,389	256,535	208.150	68,027
2900	20.920	54,480	256,648	208.884	61,292
3000	20.944	56,574	256,753	209.593	54,554
3100	20.970	58,669	256,852	210.280	47,812
3200	20.998	60,768	256,945	210.947	41,068
3300	21.028	62,869	257,032	211.593	34,320
3400	21.061	64,973	257,114	212.221	27,570
3500	21.095	67,081	257,192	212.832	20,818
3600	21.132	69,192	257,265	213.427	14,063
3700	21.171	71,308	257,334	214.007	7,307
3800	21.212	73,427	257,400	214.572	548
3900	21.254	75,550	257,462	215.123	-6,212
4000	21.299	77,678	257,522	215.662	-12,974
4100	21.345	79,810	257,579	216.189	-19,737
4200	21.392	81,947	257,635	216.703	-26,501
4300	21.441	84,088	257,688	217.207	-33,267
4400	21.490	86,235	257,740	217.701	-40,034
4500	21.541	88,386	257,790	218.184	-46,802
4600	21.593	90,543	257,840	218.658	-53,571
4700	21.646	92,705	257,889	219.123	-60,342
4800	21.699	94,872	257,938	219.580	-67,113
4900	21.752	97,045	257,987	220.028	-73,886
5000	21.805	99,223	258,036	220.468	-80,659

Table A.13 Curvfit coefficients for thermodynamic properties (C–H–O–N system)

$$\begin{aligned}\bar{c}_p/R_u &= \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 \\ \bar{h}^\circ/R_u T &= \alpha_1 + \frac{\alpha_2}{2} T + \frac{\alpha_3}{3} T^2 + \frac{\alpha_4}{4} T^3 + \frac{\alpha_5}{5} T^4 + \frac{\alpha_6}{T} \\ \bar{s}^\circ/R_u &= \alpha_1 \ln T + \alpha_2 T + \frac{\alpha_3}{2} T^2 + \frac{\alpha_4}{3} T^3 + \frac{\alpha_5}{4} T^4 + \alpha_7\end{aligned}$$

Species	T (K)	a ₁	a ₂	a ₃	a ₄	a ₅	a ₆	a ₇
CO	1000–5000	0.03025078E+02	0.14426885E–02	–0.05630827E–05	0.10185813E–09	–0.06910951E–13	–0.14268350E+05	0.06108217E+02
	300–1000	0.03262451E+02	0.15119409E–02	–0.03881755E–04	0.05581944E–07	–0.02474951E–10	–0.14310539E+05	0.04848897E+02
CO ₂	1000–5000	0.04453623E+02	0.03140168E–01	–0.12784105E–05	0.02393996E–08	–0.16690333E–13	–0.04896696E+06	–0.09553959E+01
	300–1000	0.02275724E+02	0.09922072E–01	–0.10409113E–04	0.06866686E–07	–0.02117280E–10	–0.04837314E+06	0.10188488E+02
H ₂	1000–5000	0.02991423E+02	0.07000644E–02	–0.05633828E–06	–0.09231578E–10	0.15827519E–14	–0.08350340E+04	–0.13551101E+01
	300–1000	0.03298124E+02	0.08249441E–02	–0.08143015E–05	–0.09475434E–09	0.04134872E–11	–0.10125209E+04	–0.03294094E+02
H	1000–5000	0.02500000E+02	0.00000000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.02547162E+06	–0.04601176E+01
	300–1000	0.02500000E+02	0.00000000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.02547162E+06	–0.04601176E+01
OH	1000–5000	0.02882730E+02	0.10139743E–02	–0.02276877E–05	0.02174683E–09	–0.05126303E–14	0.03886888E+05	0.05595712E+02
	300–1000	0.03637266E+02	0.01850910E–02	–0.16761646E–05	0.02387202E–07	–0.08431442E–11	0.03606781E+05	0.13588603E+01
H ₂ O	1000–5000	0.02672145E+02	0.03056293E–01	–0.08730260E–05	0.12009964E–09	–0.06391618E–13	–0.02989921E+06	0.06862817E+02
	300–1000	0.03386842E+02	0.03474982E–01	–0.06354696E–04	0.06968581E–07	–0.02506588E–10	–0.03020811E+06	0.02590232E+02
N ₂	1000–5000	0.02926640E+02	0.14879768E–02	–0.05684760E–05	0.10097038E–09	–0.06753351E–13	–0.09227977E+04	0.05980528E+02
	300–1000	0.03298677E+02	0.14082404E–02	–0.03963222E–04	0.05641515E–07	–0.02444854E–10	–0.10208999E+04	0.03950372E+02
N	1000–5000	0.02450268E+02	0.10661458E–03	–0.07465337E–06	0.01879652E–09	–0.10259839E–14	0.05611604E+06	0.04448758E+02
	300–1000	0.02503071E+02	–0.02180018E–03	0.05420529E–06	–0.05647560E–09	0.02099904E–12	0.05609890E+06	0.04167566E+02
NO	1000–5000	0.03245435E+02	0.12691383E–02	–0.05015890E–05	0.09169283E–09	–0.06275419E–13	0.09800840E+05	0.06417293E+02
	300–1000	0.03376541E+02	0.12530634E–02	–0.03302750E–04	0.05217810E–07	–0.02446262E–10	0.09817961E+05	0.05829590E+02
NO ₂	1000–5000	0.04682859E+02	0.02462429E–01	–0.10422585E–05	0.01976902E–08	–0.13917168E–13	0.02261292E+05	0.09885985E+01
	300–1000	0.02670600E+02	0.07838500E–01	–0.08063864E–04	0.06161714E–07	–0.02320150E–10	0.02896290E+05	0.11612071E+02
O ₂	1000–5000	0.03697578E+02	0.06135197E–02	–0.12588420E–06	0.01775281E–09	–0.11364354E–14	–0.12339301E+04	0.03189165E+02
	300–1000	0.03212936E+02	0.11274864E–02	–0.05756150E–05	0.13138773E–08	–0.08768554E–11	–0.10052490E+04	0.06034737E+02
O	1000–5000	0.02542059E+02	–0.02755061E–03	–0.03102803E–07	0.04551067E–10	–0.04368051E–14	0.02923080E+06	0.04920308E+02
	300–1000	0.02946428E+02	–0.16381665E–02	0.02421031E–04	–0.16028431E–08	0.03890696E–11	0.02914764E+06	0.02963995E+02

SOURCE: Kee, R. J., Rupley, F. M., and Miller, J. A., "The Chemkin Thermodynamic Data Base," Sandia Report, SAND87-8215B, reprinted March 1991.

Appendix

B

Fuel Properties

Table B.1 Selected properties of hydrocarbon fuels: enthalpy of formation,^a Gibbs function of formation,^a entropy,^a and higher and lower heating values all at 298.15 K and 1 atm; boiling points^b and latent heat of vaporization^c at 1 atm; constant-pressure adiabatic flame temperature at 1 atm,^d liquid density^c

Formula	Fuel	MW (kg/kmol)	$\bar{h}_f^\circ$ (kJ/kmol)	$\bar{g}_f^\circ$ (kJ/kmol)	$\bar{s}^\circ$ (kJ/kmol-K)	HHV [†] (kJ/kg)	LHV [†] (kJ/kg)	Boiling pt. (°C)	h_{fg} (kJ/kg)	T_{ad}^* (K)	ρ_{liq}^* (kg/m ³)
CH ₄	Methane	16.043	-74,831	-50,794	186.188	55,528	50,016	-164	509	2226	300
C ₂ H ₂	Acetylene	26.038	226,748	209,200	200.819	49,923	48,225	-84	—	2539	—
C ₂ H ₄	Ethene	28.054	52,283	68,124	219.827	50,313	47,161	-103.7	—	2369	—
C ₂ H ₆	Ethane	30.069	-84,667	-32,886	229.492	51,901	47,489	-88.6	488	2259	370
C ₃ H ₆	Propene	42.080	20,414	62,718	266.939	48,936	45,784	-47.4	437	2334	514
C ₃ H ₈	Propane	44.096	-103,847	-23,489	269.910	50,368	46,357	-42.1	425	2267	500
C ₄ H ₈	1-Butene	56.107	1,172	72,036	307.440	48,471	45,319	-63	391	2322	595
C ₄ H ₁₀	<i>n</i> -Butane	58.123	-124,733	-15,707	310.034	49,546	45,742	-0.5	386	2270	579
C ₅ H ₁₀	1-Pentene	70.134	-20,920	78,605	347.607	48,152	45,000	30	358	2314	641
C ₅ H ₁₂	<i>n</i> -Pentane	72.150	-146,440	-8,201	348.402	49,032	45,355	36.1	358	2272	626
C ₆ H ₆	Benzene	78.113	82,927	129,658	269.199	42,277	40,579	80.1	393	2342	879
C ₆ H ₁₂	1-Hexene	84.161	-41,673	87,027	385.974	47,955	44,803	63.4	335	2308	673
C ₆ H ₁₄	<i>n</i> -Hexane	86.177	-167,193	209	386.811	48,696	45,105	69	335	2273	659
C ₇ H ₁₄	1-Heptene	98.188	-62,132	95,563	424.383	47,817	44,665	93.6	—	2305	—
C ₇ H ₁₆	<i>n</i> -Heptane	100.203	-187,820	8,745	425.262	48,456	44,926	98.4	316	2274	684
C ₈ H ₁₆	1-Octene	112.214	-82,927	104,140	462.792	47,712	44,560	121.3	—	2302	—
C ₈ H ₁₈	<i>n</i> -Octane	114.230	-208,447	17,322	463.671	48,275	44,791	125.7	300	2275	703
C ₉ H ₁₈	1-Nonene	126.241	-103,512	112,717	501.243	47,631	44,478	—	—	2300	—
C ₉ H ₂₀	<i>n</i> -Nonane	128.257	-229,032	25,857	502.080	48,134	44,686	150.8	295	2276	718
C ₁₀ H ₂₀	1-Decene	140.268	-124,139	121,294	539.652	47,565	44,413	170.6	—	2298	—
C ₁₀ H ₂₂	<i>n</i> -Decane	142.284	-249,659	34,434	540.531	48,020	44,602	174.1	277	2277	730
C ₁₁ H ₂₂	1-Undecene	154.295	-144,766	129,830	578.061	47,512	44,360	—	—	2296	—
C ₁₁ H ₂₄	<i>n</i> -Undecane	156.311	-270,286	43,012	578.940	47,926	44,532	195.9	265	2277	740
C ₁₂ H ₂₄	1-Dodecene	168.322	-165,352	138,407	616.471	47,468	44,316	213.4	—	2295	—
C ₁₂ H ₂₆	<i>n</i> -Dodecane	170.337	-292,162	—	—	47,841	44,467	216.3	256	2277	749

[†]Based on gaseous fuel.

[‡]For stoichiometric combustion with air (79 percent N₂, 21 percent O₂).

^{*}For liquids at 20°C or for gases at the boiling point of the liquefied gas.

SOURCES:

^aRossini, F. D., et al., *Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds*, Carnegie Press, Pittsburgh, PA, 1953.

^bWeast, R. C. (ed.), *Handbook of Chemistry and Physics*, 56th Ed., CRC Press, Cleveland, OH, 1976.

^cObert, E. F., *Internal Combustion Engines and Air Pollution*, Harper & Row, New York, 1973.

^dCalculated using HPFLAME (Appendix F).

Table B.2 Curvefit coefficients for fuel specific heat and standardized enthalpy^a for reference state of zero enthalpy of the elements at 298.15 K, 1 atm

$$\bar{c}_p(\text{kJ/kmol}\cdot\text{K}) = 4.184 (a_1 + a_2\theta + a_3\theta^2 + a_4\theta^3 + a_5\theta^{-2}),$$

$$\bar{h}^\circ(\text{kJ/kmol}) = 4184 (a_0\theta + a_2\theta^2/2 + a_3\theta^3/3 + a_4\theta^4/4 - a_5\theta^{-1} + a_6),$$

where $\theta \equiv T(\text{K})/1000$

Formula	Fuel	MW	a_1	a_2	a_3	a_4	a_5	a_6	a_8^b
CH ₄	Methane	16.043	-0.29149	26.327	-10.610	1.5656	0.16573	-18.331	4.300
C ₃ H ₈	Propane	44.096	-1.4867	74.339	-39.065	8.0543	0.01219	-27.313	8.852
C ₆ H ₁₄	Hexane	86.177	-20.777	210.48	-164.125	52.832	0.56635	-39.836	15.611
C ₈ H ₁₈	Isooctane	114.230	-0.55313	181.62	-97.787	20.402	-0.03095	-60.751	20.232
CH ₃ OH	Methanol	32.040	-2.7059	44.168	-27.501	7.2193	0.20299	-48.288	5.3375
C ₂ H ₅ OH	Ethanol	46.07	6.990	39.741	-11.926	0	0	-60.214	7.6135
C _{8,26} H _{15,5}	Gasoline	114.8	-24.078	256.63	-201.68	64.750	0.5808	-27.562	17.792
C _{7,76} H _{13,1}		106.4	-22.501	227.99	-177.26	56.048	0.4845	-17.578	15.232
C _{10,8} H _{18,7}	Diesel	148.6	-9.1063	246.97	-143.74	32.329	0.0518	-50.128	23.514

^aSOURCE: From Heywood, J. B., *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, 1988, by permission of McGraw-Hill, Inc.

^bTo obtain 0 K reference state for enthalpy, add a_8 to a_6 .

Table B.3 Curvfit coefficients for fuel vapor thermal conductivity, viscosity, and specific heat^a

$\left[\begin{array}{l} k(\text{W/m}\cdot\text{K}) \\ \mu(\text{N}\cdot\text{s}/\text{m}^2) \cdot 10^6 \\ c_p(\text{J}/\text{kg}\cdot\text{K}) \end{array} \right] = \alpha_1 + \alpha_2 T + \alpha_3 T^2 + \alpha_4 T^3 + \alpha_5 T^4 + \alpha_6 T^5 + \alpha_7 T^6$											
Formula	Fuel	T-range (K)	Property	a_1	a_2	a_3	a_4	a_5	a_6	a_7	
CH ₄	Methane	100–1000	k	-1.34014990E-2	3.66307060E-4	-1.82248608E-6	5.93987998E-9	-9.14055050E-12	6.78968890E-15	-1.95048736E-18	
		70–1000	μ	2.96826700E-1	3.71120100E-2	1.21829800E-5	-7.02426000E-8	7.54326900E-11	-2.72371660E-14	0	
			c_p	See Table B.2							
C ₃ H ₈	Propane	200–500	k	-1.07682209E-2	8.38590325E-5	4.22059864E-8	0	0	0	0	
		270–600	μ	-3.54371100E-1	3.08096600E-2	-6.99723000E-6	0	0	0	0	
			c_p	See Table B.2							
C ₆ H ₁₄	<i>n</i> -Hexane	150–1000	k	1.28775700E-3	-2.00499443E-5	2.37858831E-7	-1.60944555E-10	7.71027290E-14	0	0	
		270–900	μ	1.54541200E+0	1.15080900E-2	2.72216500E-5	-3.26900000E-8	1.24545900E-11	0	0	
			c_p	See Table B.2							
C ₇ H ₁₆	<i>n</i> -Heptane	250–1000	k	-4.60614700E-2	5.95652224E-4	-2.98893153E-6	8.44612876E-9	-1.22927E-11	9.0127E-15	-2.62961E-18	
		270–580	μ	1.54009700E+0	1.09515700E-2	1.80066400E-5	-1.36379000E-8	0	0	0	
		300–755	c_p	9.46260000E+1	5.86099700E+0	-1.98231320E-3	-6.88699300E-8	-1.93795260E-10	0	0	
		755–1365	c_p	-7.40308000E+2	1.08935370E+1	1.26512400E-2	9.84376300E-6	-4.32282960E-9	7.86366500E-13	0	
C ₈ H ₁₈	<i>n</i> -Octane	250–500	k	-4.01391940E-3	3.38796092E-5	8.19291819E-8	0	0	0	0	
		300–650	μ	8.32435400E-1	1.40045000E-2	8.79376500E-6	-6.84030000E-9	0	0	0	
		275–755	c_p	2.14419800E+2	5.35690500E+0	-1.17497000E-3	-6.99115500E-7	0	0	0	
		755–1365	c_p	2.43596860E+3	-4.46819470E+0	1.66843290E-2	-1.78856050E-5	8.64282020E-9	-1.61426500E-12	0	
C ₁₀ H ₂₂	<i>n</i> -Decane	250–500	k	-5.88274000E-3	3.72449646E-5	7.55109624E-8	0	0	0	0	
			μ	Not available							
CH ₃ OH	Methanol	300–700	c_p	2.40717800E+2	5.09965000E+0	-6.29026000E-4	-1.07155000E-6	0	0	0	
		700–1365	c_p	-1.35345890E+4	9.14879000E+1	-2.20700000E-1	2.91406000E-4	-2.15307400E-7	8.38600000E-11	-1.34404000E-14	
		300–550	k	-2.02986750E-2	1.21910927E-4	-2.23748473E-8	0	0	0	0	
250–650	μ	1.19790000E+0	2.45028000E-2	1.86162740E-5	-1.30674820E-8	0	0	0	0		
	c_p	See Table B.2									
C ₂ H ₅ OH	Ethanol	250–550	k	-2.46663000E-2	1.55892550E-4	-8.22954822E-8	0	0	0	0	
		270–600	μ	-6.33595000E-2	3.20713470E-2	-6.25079576E-6	0	0	0	0	
			c_p	See Table B.2							

^aSOURCE: Andrews, J. R., and Bibratz, O., "Temperature Dependence of Gas Properties in Polynomial Form," Naval Postgraduate School, NPS67-81-001, January 1981.

Appendix

C

Selected Properties of Air, Nitrogen,
and Oxygen

Table C.1 Selected properties of air at 1 atm^a

T (K)	ρ (kg/m ³)	c_p (kJ/kg-K)	$\mu \cdot 10^7$ (N-s/m ²)	$\nu \cdot 10^6$ (m ² /s)	$k \cdot 10^3$ (W/m-K)	$\alpha \cdot 10^6$ (m ² /s)	Pr
100	3.5562	1.032	71.1	2.00	9.34	2.54	0.786
150	2.3364	1.012	103.4	4.426	13.8	5.84	0.758
200	1.7458	1.007	132.5	7.590	18.1	10.3	0.737
250	1.3947	1.006	159.6	11.44	22.3	15.9	0.720
300	1.1614	1.007	184.6	15.89	26.3	22.5	0.707
350	0.9950	1.009	208.2	20.92	30.0	29.9	0.700
400	0.8711	1.014	230.1	26.41	33.8	38.3	0.690
450	0.7740	1.021	250.7	32.39	37.3	47.2	0.686
500	0.6964	1.030	270.1	38.79	40.7	56.7	0.684
550	0.6329	1.040	288.4	45.57	43.9	66.7	0.683
600	0.5804	1.051	305.8	52.69	46.9	76.9	0.685
650	0.5356	1.063	322.5	60.21	49.7	87.3	0.690
700	0.4975	1.075	338.8	68.10	52.4	98.0	0.695
750	0.4643	1.087	354.6	76.37	54.9	109	0.702
800	0.4354	1.099	369.8	84.93	57.3	120	0.709
850	0.4097	1.110	384.3	93.80	59.6	131	0.716
900	0.3868	1.121	398.1	102.9	62.0	143	0.720
950	0.3666	1.131	411.3	112.2	64.3	155	0.723
1000	0.3482	1.141	424.4	121.9	66.7	168	0.726
1100	0.3166	1.159	449.0	141.8	71.5	195	0.728
1200	0.2902	1.175	473.0	162.9	76.3	224	0.728
1300	0.2679	1.189	496.0	185.1	82	238	0.719
1400	0.2488	1.207	530	213	91	303	0.703
1500	0.2322	1.230	557	240	100	350	0.685
1600	0.2177	1.248	584	268	106	390	0.688
1700	0.2049	1.267	611	298	113	435	0.685
1800	0.1935	1.286	637	329	120	482	0.683
1900	0.1833	1.307	663	362	128	534	0.677
2000	0.1741	1.337	689	396	137	589	0.672
2100	0.1658	1.372	715	431	147	646	0.667
2200	0.1582	1.417	740	468	160	714	0.655
2300	0.1513	1.478	766	506	175	783	0.647
2400	0.1448	1.558	792	547	196	869	0.630
2500	0.1389	1.665	818	589	222	960	0.613
3000	0.1135	2.726	955	841	486	1,570	0.536

^aSOURCE: Incropera, F. P., and DeWitt, D. P., *Fundamentals of Heat and Mass Transfer*, 3rd Ed. Reprinted by permission, © 1990, John Wiley & Sons, Inc.

Table C.2 Selected properties of nitrogen and oxygen at 1 atm^a

T (K)	ρ (kg/m ³)	c_p (kJ/kg-K)	$\mu \cdot 10^7$ (N-s/m ²)	$\nu \cdot 10^6$ (m ² /s)	$k \cdot 10^3$ (W/m-K)	$\alpha \cdot 10^6$ (m ² /s)	Pr
<i>Nitrogen (N₂)</i>							
100	3.4388	1.070	68.8	2.00	9.58	2.60	0.768
150	2.2594	1.050	100.6	4.45	13.9	5.86	0.759
200	1.6883	1.043	129.2	7.65	18.3	10.4	0.736
250	1.3488	1.042	154.9	11.48	22.2	15.8	0.727
300	1.1233	1.041	178.2	15.86	25.9	22.1	0.716
350	0.9625	1.042	200.0	20.78	29.3	29.2	0.711
400	0.8425	1.045	220.4	26.16	32.7	37.1	0.704
450	0.7485	1.050	239.6	32.01	35.8	45.6	0.703
500	0.6739	1.056	257.7	38.24	38.9	54.7	0.700
550	0.6124	1.065	274.7	44.86	41.7	63.9	0.702
600	0.5615	1.075	290.8	51.79	44.6	73.9	0.701
700	0.4812	1.098	321.0	66.71	49.9	94.4	0.706
800	0.4211	1.22	349.1	82.90	54.8	116	0.715
900	0.3743	1.146	375.3	100.3	59.7	139	0.721
1000	0.3368	1.167	399.9	118.7	64.7	165	0.721
1100	0.3062	1.187	423.2	138.2	70.0	193	0.718
1200	0.2807	1.204	445.3	158.6	75.8	224	0.707
1300	0.2591	1.219	466.2	179.9	81.0	256	0.701
<i>Oxygen (O₂)</i>							
100	3.945	0.962	76.4	1.94	9.25	2.44	0.796
150	2.585	0.921	114.8	4.44	13.8	5.80	0.766
200	1.930	0.915	147.5	7.64	18.3	10.4	0.737
250	1.542	0.915	178.6	11.58	22.6	16.0	0.723
300	1.284	0.920	207.2	16.14	26.8	22.7	0.711
350	1.100	0.929	233.5	21.23	29.6	29.0	0.733
400	0.9620	0.942	258.2	26.84	33.0	36.4	0.737
450	0.8554	0.956	281.4	32.90	36.3	44.4	0.741
500	0.7698	0.972	303.3	39.40	41.2	55.1	0.716
550	0.6998	0.988	324.0	46.30	44.1	63.8	0.726
600	0.6414	1.003	343.7	53.59	47.3	73.5	0.729
700	0.5498	1.031	380.8	69.26	52.8	93.1	0.744
800	0.4810	1.054	415.2	86.32	58.9	116	0.743
900	0.4275	1.074	447.2	104.6	64.9	141	0.740
1000	0.3848	1.090	477.0	124.0	71.0	169	0.733
1100	0.3498	1.103	505.5	144.5	75.8	196	0.736
1200	0.3206	1.115	532.5	166.1	81.9	229	0.725
1300	0.2960	1.125	588.4	188.6	87.1	262	0.721

^aSOURCE: Incropera, F. P., and DeWitt, D. P., *Fundamentals of Heat and Mass Transfer*, 3rd Ed. Reprinted by permission, © 1990 John Wiley & Sons, Inc.

Appendix

D

Binary Diffusion Coefficients and Methodology for their Estimation

Table D.1 Binary diffusion coefficients at 1 atm^{a,b}

Substance A	Substance B	<i>T</i> (K)	$\mathcal{D}_{AB} \cdot 10^5$ (m ² /s)
Benzene	Air	273	0.77
Carbon dioxide	Air	273	1.38
Carbon dioxide	Nitrogen	293	1.63
Cyclohexane	Air	318	0.86
<i>n</i> -Decane	Nitrogen	363	0.84
<i>n</i> -Dodecane	Nitrogen	399	0.81
Ethanol	Air	273	1.02
<i>n</i> -Hexane	Nitrogen	288	0.757
Hydrogen	Air	273	6.11
Methanol	Air	273	1.32
<i>n</i> -Octane	Air	273	0.505
<i>n</i> -Octane	Nitrogen	303	0.71
Toluene	Air	303	0.88
2,2,4-Trimethyl pentane (Isooctane)	Nitrogen	303	0.705
2,2,3-Trimethyl heptane	Nitrogen	363	0.684
Water	Air	273	2.2

^aSOURCE: Perry, R. H., Green, D. W., and Maloney, J. O., *Perry's Chemical Engineers' Handbook*, 6th Ed., McGraw-Hill, New York, 1984.

^bAssuming ideal-gas behavior, the pressure and temperature dependence of the binary diffusion coefficient can be estimated using $\mathcal{D}_{AB} \propto T^{3/2}/P$.