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## APPENDIX

# A

### SELECTED THERMODYNAMIC PROPERTIES OF GASES COMPRISING C-H-O-N SYSTEM

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#### 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.

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#### 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

$T(K)$	$\bar{c}_p$ (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
1,000	33.255	21,697	-112,022	234.450	-200,238
1,100	33.725	25,046	-112,619	237.642	-209,030
1,200	34.148	28,440	-113,240	240.595	-217,768
1,300	34.530	31,874	-113,881	243.344	-226,453
1,400	34.872	35,345	-114,543	245.915	-235,087
1,500	35.178	38,847	-115,225	248.332	-243,674
1,600	35.451	42,379	-115,925	250.611	-252,214
1,700	35.694	45,937	-116,644	252.768	-260,711
1,800	35.910	49,517	-117,380	254.814	-269,164
1,900	36.101	53,118	-118,132	256.761	-277,576
2,000	36.271	56,737	-118,902	258.617	-285,948
2,100	36.421	60,371	-119,687	260.391	-294,281
2,200	36.553	64,020	-120,488	262.088	-302,576
2,300	36.670	67,682	-121,305	263.715	-310,835
2,400	36.774	71,354	-122,137	265.278	-319,057
2,500	36.867	75,036	-122,984	266.781	-327,245
2,600	36.950	78,727	-123,847	268.229	-335,399
2,700	37.025	82,426	-124,724	269.625	-343,519
2,800	37.093	86,132	-125,616	270.973	-351,606
2,900	37.155	89,844	-126,523	272.275	-359,661
3,000	37.213	93,562	-127,446	273.536	-367,684
3,100	37.268	97,287	-128,383	274.757	-375,677
3,200	37.321	101,016	-129,335	275.941	-383,639
3,300	37.372	104,751	-130,303	277.090	-391,571
3,400	37.422	108,490	-131,285	278.207	-399,474
3,500	37.471	112,235	-132,283	279.292	-407,347
3,600	37.521	115,985	-133,295	280.349	-415,192
3,700	37.570	119,739	-134,323	281.377	-423,008
3,800	37.619	123,499	-135,366	282.380	-430,796
3,900	37.667	127,263	-136,424	283.358	-438,557
4,000	37.716	131,032	-137,497	284.312	-446,291
4,100	37.764	134,806	-138,585	285.244	-453,997
4,200	37.810	138,585	-139,687	286.154	-461,677
4,300	37.855	142,368	-140,804	287.045	-469,330
4,400	37.897	146,156	-141,935	287.915	-476,957
4,500	37.936	149,948	-143,079	288.768	-484,558
4,600	37.970	153,743	-144,236	289.602	-492,134
4,700	37.998	157,541	-145,407	290.419	-499,684

**Table A.1** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	38.019	161,342	-146,589	291.219	-507,210
4,900	38.031	165,145	-147,783	292.003	-514,710
5,000	38.033	168,948	-148,987	292.771	-522,186

**Table A.2** Carbon dioxide (CO<sub>2</sub>), 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
1,000	54.360	33,425	-394,659	269.268	-395,939
1,100	55.333	38,911	-394,875	274.495	-396,056
1,200	56.205	44,488	-395,083	279.348	-396,155
1,300	56.984	50,149	-395,287	283.878	-396,236
1,400	57.677	55,882	-395,488	288.127	-396,301
1,500	58.292	61,681	-395,691	292.128	-396,352
1,600	58.836	67,538	-395,897	295.908	-396,389
1,700	59.316	73,446	-396,110	299.489	-396,414
1,800	59.738	79,399	-396,332	302.892	-396,425
1,900	60.108	85,392	-396,564	306.132	-396,424
2,000	60.433	91,420	-396,808	309.223	-396,410
2,100	60.717	97,477	-397,065	312.179	-396,384
2,200	60.966	103,562	-397,338	315.009	-396,346
2,300	61.185	109,670	-397,626	317.724	-396,294
2,400	61.378	115,798	-397,931	320.333	-396,230
2,500	61.548	121,944	-398,253	322.842	-396,152
2,600	61.701	128,107	-398,594	325.259	-396,061
2,700	61.839	134,284	-398,952	327.590	-395,957
2,800	61.965	140,474	-399,329	329.841	-395,840
2,900	62.083	146,677	-399,725	332.018	-395,708
3,000	62.194	152,891	-400,140	334.124	-395,562
3,100	62.301	159,116	-400,573	336.165	-395,403
3,200	62.406	165,351	-401,025	338.145	-395,229
3,300	62.510	171,597	-401,495	340.067	-395,041
3,400	62.614	177,853	-401,983	341.935	-394,838
3,500	62.718	184,120	-402,489	343.751	-394,620
3,600	62.825	190,397	-403,013	345.519	-394,388
3,700	62.932	196,685	-403,553	347.242	-394,141
3,800	63.041	202,983	-404,110	348.922	-393,879
3,900	63.151	209,293	-404,684	350.561	-393,602
4,000	63.261	215,613	-405,273	353.161	-393,311
4,100	63.369	221,945	-405,878	355.725	-393,004
4,200	63.474	228,287	-406,499	355.253	-392,683
4,300	63.575	234,640	-407,135	356.748	-392,346
4,400	63.669	241,002	-407,785	358.210	-391,995
4,500	63.753	247,373	-408,451	359.642	-391,629
4,600	63.825	253,752	-409,132	361.044	-391,247
4,700	63.881	260,138	-409,828	362.417	-390,851

**Table A.2** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	63.918	266,528	-410,539	363.763	-390,440
4,900	63.932	272,920	-411,267	365.081	-390,014
5,000	63.919	279,313	-412,010	366.372	-389,572

**Table A.3** Hydrogen (H<sub>2</sub>), MW = 2.016, 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	28.522	-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
1,000	30.160	20,664	0	166.106	0
1,100	30.625	23,704	0	169.003	0
1,200	31.077	26,789	0	171.687	0
1,300	31.516	29,919	0	174.192	0
1,400	31.943	33,092	0	176.543	0
1,500	32.356	36,307	0	178.761	0
1,600	32.758	39,562	0	180.862	0
1,700	33.146	42,858	0	182.860	0
1,800	33.522	46,191	0	184.765	0
1,900	33.885	49,562	0	186.587	0
2,000	34.236	52,968	0	188.334	0
2,100	34.575	56,408	0	190.013	0
2,200	34.901	59,882	0	191.629	0
2,300	35.216	63,388	0	193.187	0
2,400	35.519	66,925	0	194.692	0
2,500	35.811	70,492	0	196.148	0
2,600	36.091	74,087	0	197.558	0
2,700	36.361	77,710	0	198.926	0
2,800	36.621	81,359	0	200.253	0
2,900	36.871	85,033	0	201.542	0
3,000	37.112	88,733	0	202.796	0
3,100	37.343	92,455	0	204.017	0
3,200	37.566	96,201	0	205.206	0
3,300	37.781	99,968	0	206.365	0
3,400	37.989	103,757	0	207.496	0
3,500	38.190	107,566	0	208.600	0
3,600	38.385	111,395	0	209.679	0
3,700	38.574	115,243	0	210.733	0
3,800	38.759	119,109	0	211.764	0
3,900	38.939	122,994	0	212.774	0
4,000	39.116	126,897	0	213.762	0
4,100	39.291	130,817	0	214.730	0
4,200	39.464	134,755	0	215.679	0
4,300	39.636	138,710	0	216.609	0
4,400	39.808	142,682	0	217.522	0
4,500	39.981	146,672	0	218.419	0
4,600	40.156	150,679	0	219.300	0
4,700	40.334	154,703	0	220.165	0

**Table A.3** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	40.516	158,746	0	221.016	0
4,900	40.702	162,806	0	221.853	0
5,000	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
1,000	20.786	14,589	222,234	139.759	165,528
1,100	20.786	16,667	222,793	141.740	159,830
1,200	20.786	18,746	223,329	143.549	154,082
1,300	20.786	20,824	223,843	145.213	148,291
1,400	20.786	22,903	224,335	146.753	142,461
1,500	20.786	24,982	224,806	148.187	136,596
1,600	20.786	27,060	225,256	149.528	130,700
1,700	20.786	29,139	225,687	150.789	124,777
1,800	20.786	31,217	226,099	151.977	118,830
1,900	20.786	33,296	226,493	153.101	112,859
2,000	20.786	35,375	226,868	154.167	106,869
2,100	20.786	37,453	227,226	155.181	100,860
2,200	20.786	39,532	227,568	156.148	94,834
2,300	20.786	41,610	227,894	157.072	88,794
2,400	20.786	43,689	228,204	157.956	82,739
2,500	20.786	45,768	228,499	158.805	76,672
2,600	20.786	47,846	228,780	159.620	70,593
2,700	20.786	49,925	229,047	160.405	64,504
2,800	20.786	52,003	229,301	161.161	58,405
2,900	20.786	54,082	229,543	161.890	52,298
3,000	20.786	56,161	229,772	162.595	46,182
3,100	20.786	58,239	229,989	163.276	40,058
3,200	20.786	60,318	230,195	163.936	33,928
3,300	20.786	62,396	230,390	164.576	27,792
3,400	20.786	64,475	230,574	165.196	21,650
3,500	20.786	66,554	230,748	165.799	15,502
3,600	20.786	68,632	230,912	166.954	9,350
3,700	20.786	70,711	231,067	166.954	3,194
3,800	20.786	72,789	231,212	167.508	-2,967
3,900	20.786	74,868	231,348	168.048	-9,132
4,000	20.786	76,947	231,475	168.575	-15,299
4,100	20.786	79,025	231,594	169.088	-21,470
4,200	20.786	81,104	231,704	169.589	-27,644
4,300	20.786	83,182	231,805	170.078	-33,820
4,400	20.786	85,261	231,897	170.556	-39,998
4,500	20.786	87,340	231,981	171.023	-46,179
4,600	20.786	89,418	232,056	171.480	-52,361
4,700	20.786	91,497	232,123	171.927	-58,545



**Table A.4** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	20.786	93,575	232,180	172.364	-64,730
4,900	20.786	95,654	232,228	172.793	-70,916
5,000	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
1,000	30.682	20,928	38,220	219.635	23,392
1,100	31.186	24,022	38,039	222.583	21,918
1,200	31.662	27,164	37,867	225.317	20,460
1,300	32.114	30,353	37,704	227.869	19,017
1,400	32.540	33,586	37,548	230.265	17,585
1,500	32.943	36,860	37,397	232.524	16,164
1,600	33.323	40,174	37,252	234.662	14,753
1,700	33.682	43,524	37,109	236.693	13,352
1,800	34.019	46,910	36,969	238.628	11,958
1,900	34.337	50,328	36,831	240.476	10,573
2,000	34.635	53,776	36,693	242.245	9,194
2,100	34.915	57,254	36,555	243.942	7,823
2,200	35.178	60,759	36,416	245.572	6,458
2,300	35.425	64,289	36,276	247.141	5,099
2,400	35.656	67,843	36,133	248.654	3,746
2,500	35.872	71,420	35,986	250.114	2,400
2,600	36.074	75,017	35,836	251.525	1,060
2,700	36.263	78,634	35,682	252.890	-275
2,800	36.439	82,269	35,524	254.212	-1,604
2,900	36.604	85,922	35,360	255.493	-2,927
3,000	36.759	89,590	35,191	256.737	-4,245
3,100	36.903	93,273	35,016	257.945	-5,556
3,200	37.039	96,970	34,835	259.118	-6,862
3,300	37.166	100,681	34,648	260.260	-8,162
3,400	37.285	104,403	34,454	261.371	-9,457
3,500	37.398	108,137	34,253	262.454	-10,745
3,600	37.504	111,882	34,046	263.509	-12,028
3,700	37.605	115,638	33,831	264.538	-13,305
3,800	37.701	119,403	33,610	265.542	-14,576
3,900	37.793	123,178	33,381	266.522	-15,841
4,000	37.882	126,962	33,146	267.480	-17,100
4,100	37.968	130,754	32,903	268.417	-18,353
4,200	38.052	134,555	32,654	269.333	-19,600
4,300	38.135	138,365	32,397	270.229	-20,841
4,400	38.217	142,182	32,134	271.107	-22,076
4,500	38.300	146,008	31,864	271.967	-23,306
4,600	38.382	149,842	31,588	272.809	-24,528
4,700	38.466	153,685	31,305	273.636	-25,745

**Table A.5** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	38.552	157,536	31,017	274.446	-26,956
4,900	38.640	161,395	30,722	275.242	-28,161
5,000	38.732	165,264	30,422	276.024	-29,360

**Table A.6** Water (H<sub>2</sub>O), 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
1,000	41.315	25,993	-247,879	232.633	-192,652
1,100	42.638	30,191	-248,475	236.634	-187,100
1,200	43.874	34,518	-249,005	240.397	-181,497
1,300	45.027	38,963	-249,477	243.955	-175,852
1,400	46.102	43,520	-249,895	247.332	-170,172
1,500	47.103	48,181	-250,267	250.547	-164,464
1,600	48.035	52,939	-250,597	253.617	-158,733
1,700	48.901	57,786	-250,890	256.556	-152,983
1,800	49.705	62,717	-251,151	259.374	-147,216
1,900	50.451	67,725	-251,384	262.081	-141,435
2,000	51.143	72,805	-251,594	264.687	-135,643
2,100	51.784	77,952	-251,783	267.198	-129,841
2,200	52.378	83,160	-251,955	269.621	-124,030
2,300	52.927	88,426	-252,113	271.961	-118,211
2,400	53.435	93,744	-252,261	274.225	-112,386
2,500	53.905	99,112	-252,399	276.416	-106,555
2,600	54.340	104,524	-252,532	278.539	-100,719
2,700	54.742	109,979	-252,659	280.597	-94,878
2,800	55.115	115,472	-252,785	282.595	-89,031
2,900	55.459	121,001	-252,909	284.535	-83,181
3,000	55.779	126,563	-253,034	286.420	-77,326
3,100	56.076	132,156	-253,161	288.254	-71,467
3,200	56.353	137,777	-253,290	290.039	-65,604
3,300	56.610	143,426	-253,423	291.777	-59,737
3,400	56.851	149,099	-253,561	293.471	-53,865
3,500	57.076	154,795	-253,704	295.122	-47,990
3,600	57.288	160,514	-253,852	296.733	-42,110
3,700	57.488	166,252	-254,007	298.305	-36,226
3,800	57.676	172,011	-254,169	299.841	-30,338
3,900	57.856	177,787	-254,338	301.341	-24,446
4,000	58.026	183,582	-254,515	302.808	-18,549
4,100	58.190	189,392	-254,699	304.243	-12,648
4,200	58.346	195,219	-254,892	305.647	-6,742
4,300	58.496	201,061	-255,093	307.022	-831
4,400	58.641	206,918	-255,303	308.368	5,085
4,500	58.781	212,790	-255,522	309.688	11,005
4,600	58.916	218,674	-255,751	310.981	16,930
4,700	59.047	224,573	-255,990	312.250	22,861

**Table A.6** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	59.173	230,484	-256,239	313.494	28,796
4,900	59.295	236,407	-256,501	314.716	34,737
5,000	59.412	242,343	-256,774	315.915	40,684

**Table A.7** Nitrogen (N<sub>2</sub>), 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
1,000	32.762	21,468	0	228.087	0
1,100	33.258	24,770	0	231.233	0
1,200	33.707	28,118	0	234.146	0
1,300	34.113	31,510	0	236.861	0
1,400	34.477	34,939	0	239.402	0
1,500	34.805	38,404	0	241.792	0
1,600	35.099	41,899	0	244.048	0
1,700	35.361	45,423	0	246.184	0
1,800	35.595	48,971	0	248.212	0
1,900	35.803	52,541	0	250.142	0
2,000	35.988	56,130	0	251.983	0
2,100	36.152	59,738	0	253.743	0
2,200	36.298	63,360	0	255.429	0
2,300	36.428	66,997	0	257.045	0
2,400	36.543	70,645	0	258.598	0
2,500	36.645	74,305	0	260.092	0
2,600	36.737	77,974	0	261.531	0
2,700	36.820	81,652	0	262.919	0
2,800	36.895	85,338	0	264.259	0
2,900	36.964	89,031	0	265.555	0
3,000	37.028	92,730	0	266.810	0
3,100	37.088	96,436	0	268.025	0
3,200	37.144	100,148	0	269.203	0
3,300	37.198	103,865	0	270.347	0
3,400	37.251	107,587	0	271.458	0
3,500	37.302	111,315	0	272.539	0
3,600	37.352	115,048	0	273.590	0
3,700	37.402	118,786	0	274.614	0
3,800	37.452	122,528	0	275.612	0
3,900	37.501	126,276	0	276.586	0
4,000	37.549	130,028	0	277.536	0
4,100	37.597	133,786	0	278.464	0
4,200	37.643	137,548	0	279.370	0
4,300	37.688	141,314	0	280.257	0
4,400	37.730	145,085	0	281.123	0
4,500	37.768	148,860	0	281.972	0
4,600	37.803	152,639	0	282.802	0
4,700	37.832	156,420	0	283.616	0

**Table A.7** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	37.854	160,205	0	284.412	0
4,900	37.868	163,991	0	285.193	0
5,000	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
1,000	20.786	14,589	476,483	178.343	412,183
1,100	20.792	16,668	476,911	180.325	405,732
1,200	20.795	18,747	477,316	182.134	399,243
1,300	20.795	20,826	477,700	183.798	392,721
1,400	20.793	22,906	478,064	185.339	386,171
1,500	20.790	24,985	478,411	186.774	379,595
1,600	20.786	27,064	478,742	188.115	372,996
1,700	20.782	29,142	479,059	189.375	366,377
1,800	20.779	31,220	479,363	190.563	359,740
1,900	20.777	33,298	479,656	191.687	353,086
2,000	20.776	35,376	479,939	192.752	346,417
2,100	20.778	37,453	480,213	193.766	339,735
2,200	20.783	39,531	480,479	194.733	333,039
2,300	20.791	41,610	480,740	195.657	326,331
2,400	20.802	43,690	480,995	196.542	319,612
2,500	20.818	45,771	481,246	197.391	312,883
2,600	20.838	47,853	481,494	198.208	306,143
2,700	20.864	49,938	481,740	198.995	299,394
2,800	20.895	52,026	481,985	199.754	292,636
2,900	20.931	54,118	482,230	200.488	285,870
3,000	20.974	56,213	482,476	201.199	279,094
3,100	21.024	58,313	482,723	201.887	272,311
3,200	21.080	60,418	482,972	202.555	265,519
3,300	21.143	62,529	483,224	203.205	258,720
3,400	21.214	64,647	483,481	203.837	251,913
3,500	21.292	66,772	483,742	204.453	245,099
3,600	21.378	68,905	484,009	205.054	238,276
3,700	21.472	71,048	484,283	205.641	231,447
3,800	21.575	73,200	484,564	206.215	224,610
3,900	21.686	75,363	484,853	206.777	217,765
4,000	21.805	77,537	485,151	207.328	210,913
4,100	21.934	79,724	485,459	207.868	204,053
4,200	22.071	81,924	485,779	208.398	197,186
4,300	22.217	84,139	486,110	208.919	190,310
4,400	22.372	86,368	486,453	209.431	183,427
4,500	22.536	88,613	486,811	209.936	176,536
4,600	22.709	90,875	487,184	210.433	169,637
4,700	22.891	93,155	487,573	210.923	162,730



**Table A.8** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	23.082	95,454	487,979	211.407	155,814
4,900	23.282	97,772	488,405	211.885	148,890
5,000	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
1,000	34.076	22,241	90,443	248.462	77,778
1,100	34.483	25,669	90,465	251.729	76,510
1,200	34.850	29,136	90,486	254.745	75,241
1,300	35.180	32,638	90,505	257.548	73,970
1,400	35.474	36,171	90,520	260.166	72,697
1,500	35.737	39,732	90,532	262.623	71,423
1,600	35.972	43,317	90,538	264.937	70,149
1,700	36.180	46,925	90,539	267.124	68,875
1,800	36.364	50,552	90,534	269.197	67,601
1,900	36.527	54,197	90,523	271.168	66,327
2,000	36.671	57,857	90,505	273.045	65,054
2,100	36.797	61,531	90,479	274.838	63,782
2,200	36.909	65,216	90,447	276.552	62,511
2,300	37.008	68,912	90,406	278.195	61,243
2,400	37.095	72,617	90,358	279.772	59,976
2,500	37.173	76,331	90,303	281.288	58,711
2,600	37.242	80,052	90,239	282.747	57,448
2,700	37.305	83,779	90,168	284.154	56,188
2,800	37.362	87,513	90,089	285.512	54,931
2,900	37.415	91,251	90,003	286.824	53,677
3,000	37.464	94,995	89,909	288.093	52,426
3,100	37.511	98,744	89,809	289.322	51,178
3,200	37.556	102,498	89,701	290.514	49,934
3,300	37.600	106,255	89,586	291.670	48,693
3,400	37.643	110,018	89,465	292.793	47,456
3,500	37.686	113,784	89,337	293.885	46,222
3,600	37.729	117,555	89,203	294.947	44,992
3,700	37.771	121,330	89,063	295.981	43,766
3,800	37.815	125,109	88,918	296.989	42,543
3,900	37.858	128,893	88,767	297.972	41,325
4,000	37.900	132,680	88,611	298.931	40,110
4,100	37.943	136,473	88,449	299.867	38,900
4,200	37.984	140,269	88,283	300.782	37,693
4,300	38.023	144,069	88,112	301.677	36,491
4,400	38.060	147,873	87,936	302.551	35,292
4,500	38.093	151,681	87,755	303.407	34,098
4,600	38.122	155,492	87,569	304.244	32,908
4,700	38.146	159,305	87,379	305.064	31,721

**Table A.9** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	38.162	163,121	87,184	305.868	30,539
4,900	38.171	166,938	86,984	306.655	29,361
5,000	38.170	170,755	86,779	307.426	28,187

**Table A.10** Nitrogen dioxide (NO<sub>2</sub>), 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
1,000	52.271	32,375	32,035	293.834	95,864
1,100	52.989	37,638	32,146	298.850	102,242
1,200	53.625	42,970	32,267	303.489	108,609
1,300	54.186	48,361	32,392	307.804	114,966
1,400	54.679	53,805	32,519	311.838	121,313
1,500	55.109	59,295	32,643	315.625	127,651
1,600	55.483	64,825	32,762	319.194	133,981
1,700	55.805	70,390	32,873	322.568	140,303
1,800	56.082	75,984	32,973	325.765	146,620
1,900	56.318	81,605	33,061	328.804	152,931
2,000	56.517	87,247	33,134	331.698	159,238
2,100	56.685	92,907	33,192	334.460	165,542
2,200	56.826	98,583	33,233	337.100	171,843
2,300	56.943	104,271	33,256	339.629	178,143
2,400	57.040	109,971	33,262	342.054	184,442
2,500	57.121	115,679	33,248	344.384	190,742
2,600	57.188	121,394	33,216	346.626	197,042
2,700	57.244	127,116	33,165	348.785	203,344
2,800	57.291	132,843	33,095	350.868	209,648
2,900	57.333	138,574	33,007	352.879	215,955
3,000	57.371	144,309	32,900	354.824	222,265
3,100	57.406	150,048	32,776	356.705	228,579
3,200	57.440	155,791	32,634	358.529	234,898
3,300	57.474	161,536	32,476	360.297	241,221
3,400	57.509	167,285	32,302	362.013	247,549
3,500	57.546	173,038	32,113	363.680	253,883
3,600	57.584	178,795	31,908	365.302	260,222
3,700	57.624	184,555	31,689	366.880	266,567
3,800	57.665	190,319	31,456	368.418	272,918
3,900	57.708	196,088	31,210	369.916	279,276
4,000	57.750	201,861	30,951	371.378	285,639
4,100	57.792	207,638	30,678	372.804	292,010
4,200	57.831	213,419	30,393	374.197	298,387
4,300	57.866	219,204	30,095	375.559	304,772
4,400	57.895	224,992	29,783	376.889	311,163
4,500	57.915	230,783	29,457	378.190	317,562
4,600	57.925	236,575	29,117	379.464	323,968
4,700	57.922	242,367	28,761	380.709	330,381

**Table A.10** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	57.902	248,159	28,389	381.929	336.803
4,900	57.862	253,947	27,998	383.122	343.232
5,000	57.798	259,730	27,586	384.290	349,670

**Table A.11** Oxygen (O<sub>2</sub>), 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
1,000	34.936	22,721	0	243.507	0
1,100	35.270	26,232	0	246.852	0
1,200	35.593	29,775	0	249.935	0
1,300	35.903	33,350	0	252.796	0
1,400	36.202	36,955	0	255.468	0
1,500	36.490	40,590	0	257.976	0
1,600	36.768	44,253	0	260.339	0
1,700	37.036	47,943	0	262.577	0
1,800	37.296	51,660	0	264.701	0
1,900	37.546	55,402	0	266.724	0
2,000	37.788	59,169	0	268.656	0
2,100	38.023	62,959	0	270.506	0
2,200	38.250	66,773	0	272.280	0
2,300	38.470	70,609	0	273.985	0
2,400	38.684	74,467	0	275.627	0
2,500	38.891	78,346	0	277.210	0
2,600	39.093	82,245	0	278.739	0
2,700	39.289	86,164	0	280.218	0
2,800	39.480	90,103	0	281.651	0
2,900	39.665	94,060	0	283.039	0
3,000	39.846	98,036	0	284.387	0
3,100	40.023	102,029	0	285.697	0
3,200	40.195	106,040	0	286.970	0
3,300	40.362	110,068	0	288.209	0
3,400	40.526	114,112	0	289.417	0
3,500	40.686	118,173	0	290.594	0
3,600	40.842	122,249	0	291.742	0
3,700	40.994	126,341	0	292.863	0
3,800	41.143	130,448	0	293.959	0
3,900	41.287	134,570	0	295.029	0
4,000	41.429	138,705	0	296.076	0
4,100	41.566	142,855	0	297.101	0
4,200	41.700	147,019	0	298.104	0
4,300	41.830	151,195	0	299.087	0
4,400	41.957	155,384	0	300.050	0
4,500	42.079	159,586	0	300.994	0
4,600	42.197	163,800	0	301.921	0
4,700	42.312	168,026	0	302.829	0

**Table A.11** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	42.421	172,262	0	303.721	0
4,900	42.527	176,510	0	304.597	0
5,000	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
1,000	20.915	14,861	252,698	186.679	187,772
1,100	20.898	16,952	253,033	188.672	181,263
1,200	20.882	19,041	253,350	190.490	174,724
1,300	20.867	21,128	253,650	192.160	168,159
1,400	20.854	23,214	253,934	193.706	161,572
1,500	20.843	25,299	254,201	195.145	154,966
1,600	20.834	27,383	254,454	196.490	148,342
1,700	20.827	29,466	254,692	197.753	141,702
1,800	20.822	31,548	254,916	198.943	135,049
1,900	20.820	33,630	255,127	200.069	128,384
2,000	20.819	35,712	255,325	201.136	121,709
2,100	20.821	37,794	255,512	202.152	115,023
2,200	20.825	39,877	255,687	203.121	108,329
2,300	20.831	41,959	255,852	204.047	101,627
2,400	20.840	44,043	256,007	204.933	94,918
2,500	20.851	46,127	256,152	205.784	88,203
2,600	20.865	48,213	256,288	206.602	81,483
2,700	20.881	50,300	256,416	207.390	74,757
2,800	20.899	52,389	256,535	208.150	68,027
2,900	20.920	54,480	256,648	208.884	61,292
3,000	20.944	56,574	256,753	209.593	54,554
3,100	20.970	58,669	256,852	210.280	47,812
3,200	20.998	60,768	256,945	210.947	41,068
3,300	21.028	62,869	257,032	211.593	34,320
3,400	21.061	64,973	257,114	212.221	27,570
3,500	21.095	67,081	257,192	212.832	20,818
3,600	21.132	69,192	257,265	213.427	14,063
3,700	21.171	71,308	257,334	214.007	7,307
3,800	21.212	73,427	257,400	214.572	548
3,900	21.254	75,550	257,462	215.123	-6,212
4,000	21.299	77,678	257,522	215.662	-12,974
4,100	21.345	79,810	257,579	216.189	-19,737
4,200	21.392	81,947	257,635	216.703	-26,501
4,300	21.441	84,088	257,688	217.207	-33,267
4,400	21.490	86,235	257,740	217.701	-40,034
4,500	21.541	88,386	257,790	218.184	-46,802
4,600	21.593	90,543	257,840	218.658	-53,571
4,700	21.646	92,705	257,889	219.123	-60,342



**Table A.12** (continued)

$T(\text{K})$	$\bar{c}_p$ (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)
4,800	21.699	94,872	257,938	219.580	-67,113
4,900	21.752	97,045	257,987	220.028	-73,886
5,000	21.805	99,223	258,036	220.468	-80,659

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

$$\bar{c}_p/R_u = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\bar{h}^o/R_u T = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T}$$

$$\bar{s}^o/R_u = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7$$

Species	T(K)	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
CO	1,000–5,000	0.03025078E+02	0.14426885E–02	–0.05630827E–05	0.10185813E–09	–0.06910951E–13	–0.14268350E+05	0.06108217E+02
	300–1,000	0.03262451E+02	0.15119409E–02	–0.03881755E–04	0.05581944E–07	–0.02474951E–10	–0.14310539E+05	0.04848897E+02
CO <sub>2</sub>	1,000–5,000	0.04453623E+02	0.03140168E–01	–0.12784105E–05	0.02393996E–08	–0.16690333E–13	–0.04896696E+06	–0.09553959E+01
	300–1,000	0.02275724E+02	0.09922072E–01	–0.10409113E–04	0.06866686E–07	–0.02117280E–10	–0.04837314E+06	0.10188488E+02
H <sub>2</sub>	1,000–5,000	0.02991423E+02	0.07000644E–02	–0.05633828E–06	–0.09231578E–10	0.15827519E–14	–0.08350340E+04	–0.13551101E+01
	300–1,000	0.03298124E+02	0.08249441E–02	–0.08143015E–05	–0.09475434E–09	0.04134872E–11	–0.10125209E+04	–0.03294094E+02
H	1,000–5,000	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.02547162E+06	–0.04601176E+01
	300–1,000	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.02547162E+06	–0.04601176E+01
OH	1,000–5,000	0.02882730E+02	0.10139743E–02	–0.02276877E–05	0.02174683E–09	–0.05126305E–14	0.03886888E+05	0.05595712E+02
	300–1,000	0.03637266E+02	0.01850910E–02	–0.16761646E–05	0.02387202E–07	–0.08431442E–11	0.03606781E+05	0.13588605E+01
H <sub>2</sub> O	1,000–5,000	0.02672145E+02	0.03056293E–01	–0.08730260E–05	0.12009964E–09	–0.06391618E–13	–0.02989921E+06	0.06862817E+02
	300–1,000	0.03386842E+02	0.03474982E–01	–0.06354696E–04	0.06968581E–07	–0.02506588E–10	–0.03020811E+06	0.02590232E+02
N <sub>2</sub>	1,000–5,000	0.02926640E+02	0.14879768E–02	–0.05684760E–05	0.10097038E–09	–0.06753351E–13	–0.09227977E+04	0.05980528E+02
	300–1,000	0.03298677E+02	0.14082404E–02	–0.03963222E–04	0.05641515E–07	–0.02444854E–10	–0.10208999E+04	0.03950372E+02
N	1,000–5,000	0.02450268E+02	0.10661458E–03	–0.07465337E–06	0.01879652E–09	–0.10259839E–14	0.05611604E+06	0.04448758E+02
	300–1,000	0.02503071E+02	–0.02180018E–03	0.05420529E–06	–0.05647560E–09	0.02099904E–12	0.05609890E+06	0.04167566E+02
NO	1,000–5,000	0.03245435E+02	0.12691383E–02	–0.05015890E–05	0.09169283E–09	–0.06275419E–13	0.09800840E+05	0.06417293E+02
	300–1,000	0.03376541E+02	0.12530634E–02	–0.03302750E–04	0.05217810E–07	–0.02446262E–10	0.09817961E+05	0.05829590E+02
NO <sub>2</sub>	1,000–5,000	0.04682859E+02	0.02462429E–01	–0.10422585E–05	0.01976902E–08	–0.13917168E–13	0.02261292E+05	0.09885985E+01
	300–1,000	0.02670600E+02	0.07838500E–01	–0.08063864E–04	0.06161714E–07	–0.02320150E–10	0.02896290E+05	0.11612071E+02

**Table A.13** (continued)

Species	T(K)	$a_1$	$a_2$	$a_3$	$a_4$	$a_5$	$a_6$	$a_7$
O <sub>2</sub>	1,000-5,000	0.03697578E+02	0.06135197E-02	-0.12588420E-06	0.01775281E-09	-0.11364354E-14	-0.12339301E+04	0.03189165E+02
	300-1,000	0.03212936E+02	0.11274864E-02	-0.05756150E-05	0.13138773E-08	-0.08768554E-11	-0.10052490E+04	0.06034737E+02
O	1,000-5,000	0.02542059E+02	-0.02755061E-03	-0.03102803E-07	0.04551067E-10	-0.04368051E-14	0.02923080E+06	0.04920308E+02
	300-1,000	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.

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**A P P E N D I X**

**B**

**FUEL PROPERTIES**

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

Formula	Fuel	MW (kg/kmol)	$\bar{h}_f^\circ$ (kJ/kmol)	$\bar{g}_f^\circ$ (kJ/kmol)	$\bar{s}^\circ$ (kJ/kmol-K)	HHV <sup>†</sup> (kJ/kg)	LHV <sup>†</sup> (kJ/kg)	Boiling pt. (°C)	$h_{fg}$ (kJ/kg)	$T_{ad}^\dagger$ (K)	$\rho_{liq}^*$ (kg/m <sup>3</sup> )
CH <sub>4</sub>	Methane	16.043	-74,831	-50,794	186.188	55,528	50,016	-164	509	2,226	300
C <sub>2</sub> H <sub>2</sub>	Acetylene	26.038	226,748	209,200	200.819	49,923	48,225	-84	—	2,539	—
C <sub>2</sub> H <sub>4</sub>	Ethene	28.054	52,283	68,124	219.827	50,313	47,161	-103.7	—	2,369	—
C <sub>2</sub> H <sub>6</sub>	Ethane	30.069	-84,667	-32,886	229.492	51,901	47,489	-88.6	488	2,259	370
C <sub>3</sub> H <sub>6</sub>	Propene	42.080	20,414	62,718	266.939	48,936	45,784	-47.4	437	2,334	514
C <sub>3</sub> H <sub>8</sub>	Propane	44.096	-103,847	-23,489	269.910	50,368	46,357	-42.1	425	2,267	500
C <sub>4</sub> H <sub>8</sub>	1-Butene	56.107	1,172	72,036	307.440	48,471	45,319	-63	391	2,322	595
C <sub>4</sub> H <sub>10</sub>	<i>n</i> -Butane	58.123	-124,733	-15,707	310.034	49,546	45,742	-0.5	386	2,270	579
C <sub>5</sub> H <sub>10</sub>	1-Pentene	70.134	-20,920	78,605	347.607	48,152	45,000	30	358	2,314	641
C <sub>5</sub> H <sub>12</sub>	<i>n</i> -Pentane	72.150	-146,440	-8,201	348.402	49,032	45,355	36.1	358	2,272	626
C <sub>6</sub> H <sub>6</sub>	Benzene	78.113	82,927	129,658	269.199	42,277	40,579	80.1	393	2,342	879
C <sub>6</sub> H <sub>12</sub>	1-Hexene	84.161	-41,673	87,027	385.974	47,955	44,803	63.4	335	2,308	673
C <sub>6</sub> H <sub>14</sub>	<i>n</i> -Hexane	86.177	-167,193	209	386.811	48,696	45,105	69	335	2,273	659
C <sub>7</sub> H <sub>14</sub>	1-Heptene	98.188	-62,132	95,563	424.383	47,817	44,665	93.6	—	2,305	—
C <sub>7</sub> H <sub>16</sub>	<i>n</i> -Heptane	100.203	-187,820	8,745	425.262	48,456	44,926	98.4	316	2,274	684
C <sub>8</sub> H <sub>16</sub>	1-Octene	112.214	-82,927	104,140	462.792	47,712	44,560	121.3	—	2,302	—
C <sub>8</sub> H <sub>18</sub>	<i>n</i> -Octane	114.230	-208,447	17,322	463.671	48,275	44,791	125.7	300	2,275	703
C <sub>9</sub> H <sub>18</sub>	1-Nonene	126.241	-103,512	112,717	501.243	47,631	44,478	—	—	2,300	—
C <sub>9</sub> H <sub>20</sub>	<i>n</i> -Nonane	128.257	-229,032	25,857	502.080	48,134	44,686	150.8	295	2,276	718
C <sub>10</sub> H <sub>20</sub>	1-Decene	140.268	-124,139	121,294	539.652	47,565	44,413	170.6	—	2,298	—
C <sub>10</sub> H <sub>22</sub>	<i>n</i> -Decane	142.284	-249,659	34,434	540.531	48,020	44,602	174.1	277	2,277	730
C <sub>11</sub> H <sub>22</sub>	1-Undecene	154.295	-144,766	129,830	578.061	47,512	44,360	—	—	2,296	—
C <sub>11</sub> H <sub>24</sub>	<i>n</i> -Undecane	156.311	-270,286	43,012	578.940	47,926	44,532	195.9	265	2,277	740

**Table B.1** (continued)

Formula	Fuel	MW (kg/kmol)	$\bar{h}_f^\circ$ (kJ/kmol)	$\bar{g}_f^\circ$ (kJ/kmol)	$\bar{s}^\circ$ (kJ/kmol-K)	HHV <sup>†</sup> (kJ/kg)	LHV <sup>†</sup> (kJ/kg)	Boiling pt. (°C)	$h_{fg}$ (kJ/kg)	$T_{ad}^\dagger$ (K)	$\rho_{liq}^*$ (kg/m <sup>3</sup> )
C <sub>12</sub> H <sub>24</sub>	1-Dodecene	168.322	-165,352	138,407	616.471	47,468	44,316	213.4	—	2,295	—
C <sub>12</sub> H <sub>26</sub>	n-Dodecane	170.337	-292,162	—	—	47,841	44,467	216.3	256	2,277	749

<sup>†</sup> Based on gaseous fuel.

<sup>‡</sup> For stoichiometric combustion with air (79 percent N<sub>2</sub>, 21 percent O<sub>2</sub>).

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

SOURCES:

<sup>a</sup>Rossini, F. D., et al., *Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds*, Carnegie Press, Pittsburgh, PA, 1953.

<sup>b</sup>Weast, R. C. (ed.), *Handbook of Chemistry and Physics*, 56th Ed., CRC Press, Cleveland, OH, 1976.

<sup>c</sup>Obert, E. F., *Internal Combustion Engines and Air Pollution*, Harper & Row, New York, 1973.

<sup>d</sup>Calculated using HPFLAME (Appendix F).

**Table B.2** Curvefit coefficients for fuel specific heat and enthalpy<sup>a</sup> for reference state of zero enthalpy of the elements at 298.15 K, 1 atm

$$\begin{aligned} c_p \text{ (kJ/kmol}\cdot\text{K)} &= 4.184(a_1 + a_2\theta + a_3\theta^2 + a_4\theta^3 + a_5\theta^{-2}), \\ \bar{h}^\circ \text{ (kJ/kmol)} &= 4184(a_1\theta + a_2\theta^2/2 + a_3\theta^3/3 + a_4\theta^4/4 - a_5\theta^{-1} + a_6), \end{aligned}$$

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 <sub>4</sub>	Methane	16.043	-0.29149	26.327	-10.610	1.5656	0.16573	-18.331	4.300
C <sub>3</sub> H <sub>8</sub>	Propane	44.096	-1.4867	74.339	-39.065	8.0543	0.01219	-27.313	8.852
C <sub>6</sub> H <sub>14</sub>	Hexane	86.177	-20.777	210.48	-164.125	52.832	0.56635	-39.836	15.611
C <sub>8</sub> H <sub>18</sub>	Isooctane	114.230	-0.55313	181.62	-97.787	20.402	-0.03095	-60.751	20.232
CH <sub>3</sub> OH	Methanol	32.040	-2.7059	44.168	-27.501	7.2193	0.20299	-48.288	5.3375
C <sub>2</sub> H <sub>5</sub> OH	Ethanol	46.07	6.990	39.741	-11.926	0	0	-60.214	7.6135
C <sub>8.26</sub> H <sub>15.5</sub>	Gasoline	114.8	-24.078	256.63	-201.68	64.750	0.5808	-27.562	17.792
C <sub>7.76</sub> H <sub>13.1</sub>		106.4	-22.501	227.99	-177.26	56.048	0.4845	-17.578	15.232
C <sub>10.8</sub> H <sub>18.7</sub>	Diesel	148.6	-9.1063	246.97	-143.74	32.329	0.0518	-50.128	23.514

<sup>a</sup>SOURCE: From Heywood, J. B., *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, 1988, by permission of McGraw-Hill, Inc.

<sup>b</sup>To obtain 0 K reference state for enthalpy, add  $a_8$  to  $a_6$ .