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Ideal Gas Thermodynamic Properties for the Phenyl, Phenoxy and o-Biphenyl Radicals

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1 ENTER:

IDEAL GAS THERMODYNAMIC PROPERTIES FOR THE PHENYL, PHENOXY, AND o-BIPHENYL RADICALS

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SUMMARY

Ideal gas thermodynamic properties of the phenyl and o-biphenyl radicals, their deuterated analogs and the phenoxy radical were calculated to 5000 K using estimated vibrational frequencies and structures. The ideal gas thermodynamic properties of benzene, biphenyl, their deuterated analogs and phenol were also calculated.

INTRODUCTION

The phenyl, phenoxy, and o-biphenyl radicals are conjectured to be important species in the mechanism of soot formation (ref. 1). Consequently their thermodynamic properties are of considerable interest. Unfortunately, relatively little is known about the thermodynamic properties of radicals over an extended range of temperatures. For example, the ideal gas thermodynamic properties of the phenyl radical as a function of temperature were published only in Bahn's compilation (ref. 2). Bahn's compilation was found to include several serious errors (ref. 3) raising questions about the accuracy of the properties for all species in the compilation. On the other hand estimates given by Benson (ref. 4) do not extend outside the room temperature range. It was therefore necessary to carry out a more accurate calculation for these very important radical species. Along with the radical calculations we have calculated the properties of the related species benzene, biphenyl, and phenol.

METHOD OF ESTIMATION FOR RADICALS

The method of estimating the vibrational assignments of the radicals is based on the Forgeteg and Berces (ref. 5) procedure which has been used to estimate ideal gas thermodynamic properties for several species (refs. 6 and 7). In this method the parent molecule assignment is taken as a standard and three vibrations are eliminated for each atom missing in the radical form. In some cases where additional information is available, some of the remaining frequencies are adjusted. The moments of inertia for the radicals are calculated usually using the same values for the interatomic distances as in the parent molecule. The thermodynamic properties are then calculated from the frequencies and the moments of inertia.

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CALCULATIONS

The basic values used to calculate the ideal gas thermodynamic functions for all species are given in table I. Moments of inertia were calculated (ref. 8) from a known or assumed structure for each species. The hindering potential for internal rotation was taken as $V(\theta) = V_2(1 - \cos 2\theta)/2$. The calculations were carried out to 5000 K using the NASA Lewis PAC4 computer program (ref. 9) and results are given in table II. The tabulations include the properties of all radicals as well as their parent species.

The heat of formation of a deuterated compound at 0 K was estimated from the heat of formation of the corresponding undeuterated compound and the heats of formation of atomic hydrogen and deuterium by the approximate formula:

$$\Delta_f H_0^\circ \text{ (deuterated)} = \Delta_f H_0^\circ \text{ (undeuterated)} + n[\Delta_f H_0^\circ \text{ (D)} - \Delta_f H_0^\circ \text{(H)}] + E_0 \text{ (deuterated)} - E_0 \text{ (undeuterated)}$$

where E_0 is the zero point energy and n is the number of hydrogen atoms replaced by deuterium. The difference $[\Delta_f H_0^\circ(D) - \Delta_f H_0^\circ(H)]$ was taken as 3.770 kJ/g-mol. For the compounds in this paper,

$$E_0 = (\frac{1}{2}\sum_i \nu_i)(1.196266 \times 10^{-2}) \text{ kJ/g-mol}$$

where ν_i are the vibrational frequencies in cm^{-1}.

Specific remarks regarding the calculation of the properties for the different species are given below.

Benzene and Benzene-d_6

The vibrational frequencies used in the calculation of benzene and benzene-d_6 properties are those compiled by Shimanouchi (ref. 10). The bond lengths for benzene, 1.397 Å(C-C) and 1.084 Å(C-H), are taken from Langseth and Stoicheff (ref. 11) and the same values were used for benzene-d_6. The heat of formation at 298.15 K, $\Delta_f H_{298}^\circ$, for benzene was taken from the API Project 44 tables (ref. 12). The heat of formation of benzene-d_6 at 0 K, $\Delta_f H_0^\circ$, was calculated using the value $\Delta_f H_0^\circ = 100.312$ kJ/g-mol for benzene from table II. Our benzene properties agree quite well with the API tables (ref. 12) which go to 3000 K and with Stull's tables (ref. 13) which go only to 1500 K.

Phenyl and Phenyl-d_5 Radicals

The vibrational assignments for benzene and benzene-d_6 were used for the corresponding radicals except that three C-H vibrations were deleted in going from the parent molecule to the radical. This was accomplished by reducing the multiplicities of a C-H stretch mode (ν_{12}) and two C-H bend modes (ν_{14}, ν_{19}). Thus for the phenyl radical we deleted the frequencies 3063, 1038, and 975 while for phenyl-d_5 we removed the frequencies 2287,

814, and 795 (see table I). The moments of inertia of the radicals were calculated using the same bond lengths as in the benzene molecule. We used Benson's heat of formation at 298.15 K (ref. 4) for the phenyl radical. The heat of formation for phenyl-d_5 was calculated using $\Delta_f H_0^\circ$ = 341.912 kJ/g-mol for the phenyl radical.

Phenol

We used the phenol vibrational assignments of Bist et al. (ref. 14) as modified by Kudchadker et al. (ref. 15). Moments of inertia were calculated from the structure given by Pedersen et al. (ref. 16). We used the same barrier to internal rotation as adopted by Kudchadker et al. (ref. 15). Our ideal gas properties tend to be slightly higher than those obtained by Kudchadker et al. Actually our value of the entropy at 400 K is closer to the value calculated by Kudchadker et al. from experimental data than is the entropy of Kudchadker et al.

In order to evaluate the uncertainties in the estimating technique, the calculation of the phenyl radical was repeated but using phenol as the parent molecule. The vibrational assignments of Bist et al. (ref. 14) were used and the vibrations of OH (3656 and 1176), CO (1501), and the x-sensitive and torsion frequencies 503,309 and 244 cm^{-1} were discarded. The calculated values of the phenyl radical using the two different parent molecules compared very well. The values are well within the expected accuracy for an estimated species. A comparison of the values obtained with the two sets of vibrations is given in table III. While either set should be acceptable, we prefer those estimated from the benzene molecule for consistency with the estimates of deuterated phenyl.

Phenoxy Radical

The phenoxy radical was calculated using phenol as the parent molecule. The vibrational frequencies used for phenol were also used for phenoxy with three vibrations discarded: the OH frequencies (3656 and 1176) and the vibration of the internal rotor. The moments of inertia were calculated from the phenol structure using the same C-H and C-C bond lengths. The bond length of the C-O bond was estimated by reducing the phenol bond length by 3.5 percent. The bond angle $\angle$ OCC was taken as 120°. The heat of formation $\Delta_f H^\circ_{298}$ was taken from Colussi et al. (ref. 17). A comparison of our values with those estimated by Colussi et al. is shown in table III.

Biphenyl and Biphenyl-d_{10}

The vibrational assignments for biphenyl and biphenyl-d_{10} are those of Zerbi and Sandroni (ref. 18). Where they did not make an assignment we picked the assignments of Kovner (ref. 19) and Peregudov (ref. 20) as given by Zerbi and Sandroni in their tables 4 and 6. Any frequencies still unassigned were taken from Katon and Lippincott (ref. 21). Based on the Zerbi and Sandroni discussion it is clear that the frequency $\nu_3(B_{2g})$ given as 708 cm^{-1} in their table 4 should really be 780 cm^{-1}. The moments of inertia for both molecules were calculated with the structure adopted by Zerbi and Sandroni, due to Trotter (ref. 22), with one exception. The C-C bond length between

meta and para carbons, listed as 1.376 Å, was changed to 1.3863 Å. The value 1.376 is inadequate for ring closure if all other geometrical parameters are correct and hence is probably a typographical error and should have been 1.386 Å. The angle of ring twist is 45° as chosen by Zerbi and Sandroni. The heat of formation $\Delta_f H^\circ_{298}$ for biphenyl was taken from Cox and Pilcher (ref. 23). The barrier to internal rotation for both molecules was chosen as 1.5 kcal/g-mol. Katon and Lippincott (ref. 21) had estimated that it was between 1 and 2 kcal/g-mol while Poshkus and Grumadas estimated 1.7 kcal/g-mol (ref. 24.).

o-Biphenyl and o-Biphenyl-d_9

The biphenyl molecule was taken as the parent of the radical. Three C-H vibrations were eliminated: (3073, 1040, 969) from biphenyl and (2284, 952, 783) from biphenyl-d_{10}. The heat of formation for o-biphenyl was calculated from the heat of formation of biphenyl using a bond dissociation energy of 110.8 kcal/g-mol for the C-H bond in biphenyl. This is the same value as the bond dissociation energy for the C-H bond in benzene.

Least Squares Representation of Data

A set of least squares coefficients is presented here for the range 300 to 5000 K. The coefficients given in table IV can generate the thermodynamic properties according to the following formulas:

$$\frac{C^\circ_p}{R} = A_1 + A_2T + A_3T^2 + A_4T^3 + A_5T^4$$

$$\frac{H^\circ_T}{RT} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 + \frac{A_6}{T}$$

$$\frac{S^\circ}{R} = A_1 \ln T + A_2T + \frac{A_3}{2}T^2 + \frac{A_4}{3}T^3 + \frac{A_5}{4}T^4 + A_7$$

$$\frac{G^\circ}{RT} = A_1(1 - \ln T) - \frac{A_2}{2}T - \frac{A_3}{6}T^2 - \frac{A_4}{12}T^3 - \frac{A_5}{20}T^4 + \frac{A_6}{T} - A_7$$

For each species, starting on line 2, the first seven numbers cover the temperature interval from 1000 to 5000 K, and the next seven numbers cover the interval from 300 to 1000 K. The last number for each species in table IV is $\Delta_f H^\circ_{298}/R$ in kelvins. The last number on line 1 is the molecular weight.

ACCURACY OF CALCULATIONS

It is not possible to assess the accuracy of the estimated free radical properties with any certainty because there are no experimental thermodynamic measurements with which they might be compared. However, the consistencies in the results from different methods of estimation, shown in table III, imply that the free radical properties given in table II are probably realistic approximations to the exact values.

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TABLE I. - VIBRATIONAL FREQUENCIES AND OTHER MOLECULAR

(a) Frequencies, ν_i, cm^{-1}

i	C_6H_6	C_6H_5	C_6D_6	C_6D_5	C_6H_5OH	C_6H_5O	$C_{12}H_{10}$	$C_{12}H_9$	$C_{12}D_{10}$	$C_{12}D_9$
1	3062	3062	2293	2293	3656	----	3080	3080	2287	2287
2	992	992	943	943	3087	3087	3073	----	2284	----
3	1326	1326	1037	1037	3063	3063	3072	3072	2280	2280
4	673	673	497	497	3027	3027	1612	1612	1571	1571
5	3068	3068	2292	2292	1603	1603	1507	1507	1412	1412
6	1010	1010	969	969	1501	1501	1285	1285	1188	1188
7	995	995	827	827	1261	1261	1190	1190	960	960
8	703	703	601	601	1176	----	1030	1030	869	869
9	1310	1310	1286	1286	1168	1168	1003	1003	835	835
10	1150	1150	824	824	1025	1025	742	742	688	688
11	849(2)	849(2)	662(2)	662(2)	999	999	315	315	300	300
12	3063(2)	3063	2287(2)	2287	823	823	3069	3069	2286	2286
13	1486(2)	1486(2)	1335(2)	1335(2)	526	526	3068	3068	2218	2218
14	1038(2)	1038	814(2)	814	3070	3070	1570	1570	1531	1531
15	3047(2)	3047(2)	2265(2)	2265(2)	3049	3049	1432	1432	1328	1328
16	1596(2)	1596(2)	1552(2)	1552(2)	1610	1610	1383	1383	1266	1266
17	1178(2)	1178(2)	867(2)	867(2)	1472	1472	1283	1283	1010	1010
18	606(2)	606(2)	577(2)	577(2)	1343	1343	1156	1156	826	826
19	975(2)	975	795(2)	795	1277	1277	1074	1074	790	790
20	410(2)	410(2)	352(2)	352(2)	1150	1150	626	626	565	565
21					1070	1070	116	116	110	110
22					619	619	970	970	832	832
23					403	403	903	903	744	744
24					958	958	736	736	627	627
25					817	817	698	698	540	540
26					409	409	484	484	466	466
27					973	973	174	174	160	160
28					881	881	965	965	790	790
29					751	751	838	838	652	652
30					686	686	400	400	346	346
31					503	503	3080	3080	2288	2288
32					309[a]	----	3072	3072	2284	2284
33					225	225	3072	3072	2281	2281
34							1597	1597	1568	1568
35							1482	1482	1346	1346
36							1176	1176	983	983
37							1040	----	952	----
38							1008	1008	846	846
39							965	965	816	816
40							609	609	590	590
41							3069	3069	2285	2285
42							3068	3068	2279	2279
43							1595	1595	1566	1566
44							1452	1452	1345	1345
45							1376	1376	1272	1272
46							1316	1316	1070	1070
47							1156	1156	840	840
48							1090	1090	835	835
49							608	608	589	589
50							407	407	355	355
51							980	980	775	775
52							897	897	646	646
53							780	780	539	539
54							545	545	500	500
55							441	441	393	393
56							260	260	232	232
57							969	----	783	----
58							838	838	660	660
59							400	400	300	300
60							70[a]	----	----	----

[a]Torsion frequency, not used in calculation of properties.

(b) Other molecular properties

	C_6H_6	C_6H_5	C_6D_6	C_6D_5	C_6H_5OH	C_6H_5O	$C_{12}H_{10}$	$C_{12}H_9$	$C_{12}D_{10}$	$C_{12}D_9$
I_A, $\times 10^{-39}$ g cm^2	14.77	13.72	17.85	15.74	14.89	14.76	28.67	27.88	34.79	33.21
I_B, $\times 10^{-39}$ g cm^2	= IA	14.77	= IA	17.85	32.16	30.31	155.07	154.77	171.43	170.83
I_C, $\times 10^{-39}$ g cm^2	29.54	28.49	35.71	33.60	46.78	45.06	175.34	174.50	196.03	194.34
I_R, $\times 10^{-39}$ g cm^2	------	------	------	------	0.1336	------	7.166	6.965	8.697	8.285
$\Delta_f H^\circ_{298}$, kJ/g-mol	82.80	328.4	58.18	306.94	-96.399	47.70	182.13	727.73	138.41	386.51
Statistical wt.	1	2	1	2	1	2	1	2	1	2
V(2), cal/g-mol	------	------	------	------	3468	------	1500	1500	1500	1500
σ(int. rotation)	------	------	------	------	2	------	2	2	2	2
σ(ext. rotation)	12	2	12	2	1	2	4	1	4	1

TABLE II. - IDEAL GAS PROPERTIES

II(a) PHENYL RADICAL (C_6H_5)

T	C_p°	$H_T^\circ - H_{298.15}^\circ$	S°	$-(G_T^\circ - H_{298.15}^\circ)/T$	H_T°	$\Delta_f H_T^\circ$	$\log_{10} K$
K	J/g-mol K	kJ/g-mol	J/g-mol K	J/g-mol K	kJ/g-mol	kJ/g-mol	
0	-------	-14.005	-------	-------	314.439	341.912	-------
100	35.160	-10.648	233.879	340.363	317.796	337.417	-177.4678
200	52.345	-6.402	262.636	294.646	322.042	332.969	-89.7885
298.15	78.813	-0.000	288.328	288.328	328.444	328.444	-61.3306
300	79.338	0.146	288.817	288.329	328.590	328.354	-60.9750
400	106.601	9.467	315.444	291.775	337.911	324.290	-46.7673
500	129.812	21.327	341.811	299.157	349.771	320.880	-38.3392
600	148.562	35.280	367.198	308.399	363.724	318.047	-32.7776
700	163.683	50.919	391.275	318.535	379.363	315.698	-28.8354
800	176.051	67.925	413.966	329.060	396.369	313.797	-25.9004
900	186.314	86.059	435.313	339.692	414.503	312.268	-23.6275
1000	194.928	105.133	455.402	350.268	433.577	311.104	-21.8183
1100	202.217	125.000	474.332	360.695	453.444	310.222	-20.3442
1200	208.424	145.541	492.200	370.916	473.985	309.558	-19.1182
1300	213.737	166.656	509.098	380.902	495.100	309.062	-18.0823
1400	218.305	188.263	525.109	390.635	516.707	308.728	-17.1954
1500	222.251	210.296	540.309	400.111	538.740	308.479	-16.4279
1600	225.674	232.696	554.764	409.329	561.140	308.342	-15.7572
1700	228.656	255.416	568.537	418.292	583.860	308.219	-15.1646
1800	231.265	278.415	581.682	427.007	606.859	308.145	-14.6389
1900	233.556	301.659	594.249	435.481	630.103	308.096	-14.1684
2000	235.578	325.118	606.281	443.722	653.562	308.017	-13.7453
2100	237.367	348.766	617.819	451.740	677.210	307.944	-13.3616
2200	238.957	372.584	628.899	459.542	701.028	307.846	-13.0130
2300	240.375	396.552	639.553	467.139	724.996	307.725	-12.6965
2400	241.643	420.654	649.810	474.538	749.098	307.538	-12.4049
2500	242.783	444.877	659.698	481.748	773.321	307.349	-12.1373
2600	243.809	469.207	669.241	488.776	797.651	307.068	-11.8904
2700	244.736	493.635	678.460	495.632	822.079	306.747	-11.6622
2800	245.576	518.151	687.376	502.322	846.595	306.367	-11.4497
2900	246.340	542.748	696.007	508.852	871.192	305.938	-11.2534
3000	247.035	567.417	704.370	515.231	895.861	305.430	-11.0699
3100	247.670	592.153	712.481	521.464	920.597	304.875	-10.8984
3200	248.251	616.949	720.353	527.557	945.393	304.218	-10.7373
3300	248.785	641.801	728.001	533.516	970.245	303.524	-10.5874
3400	249.275	666.705	735.435	539.345	995.149	302.719	-10.4460
3500	249.727	691.655	742.668	545.052	1020.099	301.868	-10.3134
3600	250.145	716.649	749.708	550.639	1045.093	300.934	-10.1886
3700	250.531	741.682	756.567	556.113	1070.126	299.911	-10.0703
3800	250.889	766.754	763.253	561.476	1095.198	298.824	-9.9599
3900	251.221	791.860	769.775	566.734	1120.304	297.628	-9.8538
4000	251.530	816.998	776.139	571.890	1145.442	296.363	-9.7550
4100	251.818	842.165	782.353	576.947	1170.609	295.010	-9.6613
4200	252.086	867.360	788.425	581.911	1195.804	293.593	-9.5722
4300	252.337	892.582	794.360	586.783	1221.026	292.074	-9.4874
4400	252.572	917.828	800.164	591.566	1246.272	290.462	-9.4073
4500	252.792	943.095	805.842	596.265	1271.539	288.770	-9.3307
4600	252.999	968.386	811.400	600.882	1296.830	286.994	-9.2580
4700	253.192	993.695	816.844	605.419	1322.139	285.109	-9.1879
4800	253.375	1019.024	822.176	609.880	1347.468	283.161	-9.1219
4900	253.547	1044.370	827.402	614.266	1372.814	281.115	-9.0597
5000	253.709	1069.733	832.527	618.580	1398.177	278.993	-8.9999
5100	253.861	1095.111	837.552	622.824	1423.555	276.768	-8.9431
5200	254.006	1120.505	842.483	627.001	1448.949	274.478	-8.8889
5300	254.142	1145.912	847.323	631.113	1474.356	272.095	-8.8377
5400	254.271	1171.333	852.074	635.161	1499.777	269.608	-8.7881
5500	254.394	1196.766	856.741	639.147	1525.210	267.063	-8.7400
5600	254.510	1222.210	861.325	643.074	1550.654	264.446	-8.6952
5700	254.620	1247.667	865.832	646.943	1576.111	261.737	-8.6518
5800	254.725	1273.135	870.261	650.755	1601.579	258.966	-8.6118
5900	254.824	1298.612	874.616	654.512	1627.056	256.109	-8.5729
6000	254.919	1324.100	878.899	658.216	1652.544	253.156	-8.5348

TABLE II. - Continued.

II(b) BENZENE (C_6H_6)

T	C°_p	$H^\circ_T - H^\circ_{298.15}$	S°	$-(G^\circ_T - H^\circ_{298.15})/T$	H°_T	$\Delta_f H^\circ_T$	$\log_{10} K$
K	J/g-mol K	kJ/g-mol	J/g-mol K	J/g-mol K	kJ/g-mol	kJ/g-mol	
0	--------	-14.194	--------	--------	68.606	100.312	--------
100	35.162	-10.838	213.837	322.221	71.962	94.317	-54.1620
200	52.979	-6.575	242.694	275.567	76.225	88.539	-30.1085
298.15	81.922	-0.000	269.055	269.055	82.800	82.800	-22.7122
300	82.503	0.152	269.563	269.056	82.952	82.689	-22.6220
400	112.784	9.943	297.520	272.663	92.743	77.642	-19.1281
500	138.541	22.553	325.551	280.446	105.353	73.521	-17.1508
600	159.309	37.483	352.715	290.243	120.283	70.200	-15.9003
700	176.073	54.281	378.576	301.032	137.081	67.542	-15.0424
800	189.826	72.598	403.014	312.267	155.398	65.474	-14.4230
900	201.287	92.170	426.054	323.643	174.970	63.896	-13.9518
1000	210.949	112.795	447.776	334.980	195.595	62.781	-13.5840
1100	219.158	134.312	468.277	346.175	217.112	62.030	-13.2887
1200	226.173	156.587	487.655	357.165	239.387	61.561	-13.0446
1300	232.196	179.513	506.002	367.915	262.313	61.315	-12.8387
1400	237.389	202.999	523.405	378.405	285.799	61.278	-12.6624
1500	241.884	226.968	539.940	388.628	309.768	61.361	-12.5100
1600	245.791	251.356	555.678	398.581	334.156	61.586	-12.3767
1700	249.200	276.110	570.684	408.266	358.910	61.850	-12.2577
1800	252.186	301.182	585.014	417.691	383.982	62.182	-12.1522
1900	254.812	326.535	598.721	426.860	409.335	62.556	-12.0570
2000	257.131	352.134	611.851	435.784	434.934	62.913	-11.9711
2100	259.185	377.952	624.447	444.470	460.752	63.288	-11.8920
2200	261.011	403.964	636.547	452.928	486.764	63.643	-11.8197
2300	262.642	430.148	648.187	461.166	512.948	63.982	-11.7550
2400	264.101	456.486	659.396	469.193	539.286	64.262	-11.6940
2500	265.412	482.963	670.204	477.019	565.763	64.543	-11.6380
2600	266.594	509.564	680.637	484.651	592.364	64.734	-11.5859
2700	267.662	536.278	690.719	492.097	619.078	64.887	-11.5379
2800	268.630	563.094	700.471	499.366	645.894	64.980	-11.4923
2900	269.510	590.002	709.913	506.464	672.802	65.026	-11.4511
3000	270.312	616.993	719.064	513.399	699.793	64.992	-11.4122
3100	271.044	644.061	727.939	520.177	726.861	64.910	-11.3755
3200	271.715	671.200	736.555	526.805	754.000	64.723	-11.3406
3300	272.330	698.402	744.926	533.289	781.202	64.499	-11.3091
3400	272.897	725.665	753.064	539.634	808.465	64.159	-11.2788
3500	273.418	752.981	760.982	545.845	835.781	63.772	-11.2509
3600	273.900	780.347	768.692	551.929	863.147	63.297	-11.2247
3700	274.346	807.760	776.203	557.889	890.560	62.732	-11.1995
3800	274.760	835.215	783.525	563.731	918.015	62.095	-11.1771
3900	275.143	862.710	790.667	569.459	945.510	61.348	-11.1544
4000	275.500	890.243	797.637	575.077	973.043	60.526	-11.1347
4100	275.833	917.809	804.444	580.588	1000.609	59.611	-11.1161
4200	276.143	945.409	811.095	585.997	1028.209	58.629	-11.0983
4300	276.433	973.037	817.596	591.308	1055.837	57.539	-11.0813
4400	276.704	1000.695	823.954	596.523	1083.495	56.351	-11.0660
4500	276.959	1028.378	830.176	601.647	1111.178	55.076	-11.0510
4600	277.197	1056.086	836.265	606.681	1138.886	53.714	-11.0373
4700	277.421	1083.817	842.229	611.630	1166.617	52.236	-11.0235
4800	277.632	1111.569	848.072	616.495	1194.369	50.691	-11.0113
4900	277.831	1139.343	853.799	621.280	1222.143	49.043	-11.0007
5000	278.018	1167.135	859.414	625.987	1249.935	47.312	-10.9903
5100	278.194	1194.946	864.921	630.618	1277.746	45.475	-10.9810
5200	278.361	1222.774	870.325	635.176	1305.574	43.567	-10.9722
5300	278.519	1250.619	875.629	639.663	1333.419	41.562	-10.9648
5400	278.669	1278.478	880.836	644.081	1361.278	39.447	-10.9572
5500	278.810	1306.351	885.950	648.432	1389.151	37.271	-10.9496
5600	278.944	1334.239	890.975	652.718	1417.039	35.020	-10.9437
5700	279.072	1362.140	895.914	656.942	1444.940	32.670	-10.9378
5800	279.193	1390.054	900.768	661.104	1472.854	30.259	-10.9340
5900	279.308	1417.978	905.542	665.206	1500.778	27.757	-10.9300
6000	279.418	1445.916	910.237	669.251	1528.716	25.155	-10.9255

TABLE II. - Continued.

II(c) PHENYL RADICAL-d_5 (C_6D_5)

T	C_p°	$H_T^\circ - H_{298.15}^\circ$	S°	$-(G_T^\circ - H_{298.15}^\circ)/T$	H_T°	$\Delta_f H_T^\circ$	$\log_{10} K$
K	J/g-mol K	kJ/g-mol	J/g-mol K	J/g-mol K	kJ/g-mol	kJ/g-mol	
0	-------	-15.919	-------	-------	291.025	318.749	-------
100	36.875	-12.528	237.122	362.407	294.416	314.915	-167.1203
200	62.288	-7.728	269.391	308.030	299.217	310.373	-85.3490
298.15	94.995	-0.000	300.392	300.392	306.944	306.944	-58.7986
300	95.585	0.176	300.981	300.394	307.120	306.884	-58.4662
400	124.492	11.231	332.584	304.507	318.175	304.512	-45.1606
500	147.572	24.879	362.942	313.185	331.823	302.880	-37.2280
600	165.922	40.588	391.533	323.886	347.532	301.750	-31.9656
700	180.622	57.942	418.255	335.481	364.886	301.012	-28.2164
800	192.470	76.617	443.175	347.403	383.562	300.602	-25.4119
900	202.071	96.361	466.418	359.351	403.305	300.421	-23.2297
1000	209.895	116.972	488.127	371.155	423.917	300.470	-21.4860
1100	216.311	138.293	508.444	382.722	445.237	300.655	-20.0597
1200	221.608	160.198	527.500	394.002	467.142	300.936	-18.8699
1300	226.013	182.585	545.417	404.967	489.529	301.253	-17.8614
1400	229.701	205.376	562.305	415.608	512.320	301.632	-16.9957
1500	232.813	228.506	578.262	425.925	535.450	301.999	-16.2452
1600	235.455	251.923	593.374	435.922	558.867	302.408	-15.5886
1700	237.715	275.585	607.718	445.609	582.529	302.756	-15.0062
1800	239.659	299.456	621.362	454.997	606.400	303.094	-14.4899
1900	241.342	323.508	634.366	464.098	630.452	303.403	-14.0267
2000	242.807	347.717	646.783	472.924	654.661	303.646	-13.6098
2100	244.089	372.063	658.661	481.488	679.007	303.842	-13.2308
2200	245.217	396.529	670.043	489.802	703.474	304.005	-12.8878
2300	246.213	421.102	680.965	497.878	728.046	304.101	-12.5748
2400	247.098	445.769	691.463	505.726	752.713	304.113	-12.2861
2500	247.886	470.518	701.566	513.359	777.462	304.106	-12.0217
2600	248.592	495.343	711.303	520.786	802.287	303.985	-11.7769
2700	249.225	520.235	720.697	528.018	827.179	303.814	-11.5514
2800	249.796	545.186	729.771	535.062	852.130	303.576	-11.3407
2900	250.313	570.192	738.546	541.928	877.136	303.263	-11.1464
3000	250.781	595.247	747.040	548.624	902.191	302.858	-10.9643
3100	251.206	620.346	755.270	555.158	927.291	302.406	-10.7941
3200	251.595	645.487	763.252	561.537	952.431	301.852	-10.6347
3300	251.950	670.664	770.999	567.767	977.608	301.243	-10.4853
3400	252.276	695.876	778.526	573.856	1002.821	300.527	-10.3453
3500	252.575	721.119	785.843	579.809	1028.063	299.749	-10.2131
3600	252.850	746.390	792.962	585.631	1053.334	298.893	-10.0896
3700	253.104	771.688	799.893	591.329	1078.632	297.936	-9.9719
3800	253.339	797.011	806.646	596.907	1103.955	296.921	-9.8625
3900	253.557	822.355	813.230	602.370	1129.299	295.788	-9.7574
4000	253.759	847.721	819.652	607.722	1154.666	294.583	-9.6586
4100	253.947	873.107	825.921	612.968	1180.051	293.291	-9.5656
4200	254.123	898.511	832.042	618.111	1205.455	291.936	-9.4769
4300	254.286	923.931	838.024	623.156	1230.875	290.469	-9.3928
4400	254.438	949.367	843.871	628.106	1256.311	288.923	-9.3128
4500	254.581	974.818	849.591	632.964	1281.763	287.288	-9.2368
4600	254.715	1000.284	855.188	637.735	1307.228	285.572	-9.1647
4700	254.840	1025.761	860.667	642.420	1332.705	283.750	-9.0950
4800	254.958	1051.251	866.033	647.023	1358.195	281.860	-9.0292
4900	255.069	1076.753	871.292	651.546	1383.697	279.875	-8.9674
5000	255.174	1102.264	876.446	655.993	1409.208	277.827	-8.9075
5100	255.272	1127.787	881.500	660.365	1434.731	275.675	-8.8508
5200	255.365	1153.319	886.458	664.666	1460.263	273.460	-8.7972
5300	255.453	1178.860	891.323	668.896	1485.804	271.148	-8.7461
5400	255.536	1204.409	896.099	673.060	1511.353	268.748	-8.6968
5500	255.615	1229.967	900.788	677.158	1536.911	266.286	-8.6485
5600	255.689	1255.532	905.395	681.192	1562.477	263.758	-8.6040
5700	255.760	1281.105	909.921	685.166	1588.049	261.143	-8.5606
5800	255.827	1306.685	914.370	689.079	1613.629	258.474	-8.5206
5900	255.891	1332.270	918.743	692.935	1639.214	255.715	-8.4816
6000	255.952	1357.863	923.045	696.734	1664.807	252.887	-8.4443

TABLE II. - Continued.

II(d) BENZENE-d_6 (C_6D_6)

T	C°_p	$H^\circ_T - H^\circ_{298.15}$	S°	$-(G^\circ_T - H^\circ_{298.15})/T$	H°_T	$\Delta_f H^\circ_T$	$\log_{10} K$
K	J/g-mol K	kJ/g-mol	J/g-mol K	J/g-mol K	kJ/g-mol	kJ/g-mol	
0	-------	-16.324	-------	-------	41.853	73.861	-------
100	36.896	-12.934	217.542	346.881	45.243	68.653	-42.4534
200	64.008	-8.074	250.157	290.527	50.103	62.693	-25.1459
298.15	100.395	-0.000	282.517	282.517	58.177	58.177	-19.9330
300	101.055	0.186	283.140	282.519	58.364	58.100	-19.8694
400	133.283	11.961	316.791	286.888	70.138	54.988	-17.4087
500	158.909	26.621	349.397	296.155	84.798	52.903	-15.9990
600	179.275	43.568	380.239	307.626	101.745	51.537	-15.0913
700	195.628	62.342	409.147	320.087	120.520	50.730	-14.4543
800	208.855	82.590	436.164	332.927	140.767	50.379	-13.9842
900	219.611	104.031	461.406	345.816	162.209	50.356	-13.6168
1000	228.402	126.447	485.015	358.569	184.624	50.642	-13.3238
1100	235.629	149.660	507.134	371.080	207.837	51.123	-13.0831
1200	241.608	173.531	527.901	383.292	231.708	51.748	-12.8802
1300	246.588	197.948	547.442	395.175	256.125	52.441	-12.7054
1400	250.765	222.822	565.874	406.716	280.999	53.227	-12.5532
1500	254.292	248.079	583.298	417.912	306.257	54.021	-12.4201
1600	257.291	273.662	599.808	428.769	331.840	54.876	-12.3027
1700	259.857	299.523	615.485	439.295	357.700	55.683	-12.1953
1800	262.066	325.622	630.403	449.501	383.799	56.489	-12.1004
1900	263.980	351.927	644.624	459.400	410.104	57.275	-12.0134
2000	265.647	378.419	658.208	469.003	436.587	58.001	-11.9345
2100	267.107	405.049	671.205	478.325	463.226	58.682	-11.8607
2200	268.391	431.825	683.661	487.377	490.002	59.337	-11.7946
2300	269.526	458.722	695.617	496.173	516.900	59.925	-11.7339
2400	270.534	485.726	707.110	504.724	543.903	60.431	-11.6760
2500	271.432	512.825	718.172	513.042	571.003	60.920	-11.6236
2600	272.237	540.010	728.834	521.138	598.187	61.293	-11.5740
2700	272.959	567.270	739.122	529.022	625.447	61.616	-11.5290
2800	273.610	594.599	749.061	536.704	652.776	61.870	-11.4854
2900	274.199	621.990	758.672	544.193	680.167	62.048	-11.4463
3000	274.733	649.437	767.977	551.498	707.614	62.132	-11.4090
3100	275.219	676.935	776.994	558.628	735.112	62.165	-11.3738
3200	275.662	704.480	785.739	565.589	762.657	62.095	-11.3408
3300	276.068	732.066	794.228	572.389	790.243	61.967	-11.3098
3400	276.439	759.692	802.475	579.036	817.869	61.727	-11.2812
3500	276.781	787.353	810.493	585.535	845.530	61.421	-11.2536
3600	277.095	815.047	818.295	591.893	873.224	61.036	-11.2288
3700	277.386	842.772	825.891	598.115	900.949	60.543	-11.2043
3800	277.654	870.524	833.292	604.207	928.701	59.991	-11.1830
3900	277.903	898.302	840.507	610.174	956.479	59.313	-11.1614
4000	278.134	926.103	847.546	616.021	984.281	58.558	-11.1417
4100	278.348	953.928	854.417	621.752	1012.105	57.713	-11.1239
4200	278.548	981.773	861.127	627.371	1039.950	56.802	-11.1065
4300	278.735	1009.637	867.683	632.884	1067.814	55.770	-11.0904
4400	278.909	1037.519	874.093	638.293	1095.696	54.658	-11.0751
4500	279.072	1065.419	880.363	643.603	1123.596	53.448	-11.0607
4600	279.225	1093.334	886.499	648.817	1151.511	52.155	-11.0478
4700	279.368	1121.262	892.505	653.938	1179.439	50.749	-11.0343
4800	279.503	1149.206	898.388	658.970	1207.383	49.271	-11.0224
4900	279.630	1177.163	904.153	663.915	1235.341	47.693	-11.0122
5000	279.749	1205.131	909.803	668.776	1263.309	46.050	-11.0018
5100	279.862	1233.113	915.344	673.557	1291.290	44.295	-10.9925
5200	279.968	1261.105	920.779	678.259	1319.282	42.476	-10.9845
5300	280.068	1289.107	926.113	682.886	1347.284	40.553	-10.9771
5400	280.163	1317.118	931.349	687.438	1375.296	38.540	-10.9699
5500	280.253	1345.138	936.491	691.920	1403.315	36.460	-10.9620
5600	280.338	1373.169	941.541	696.332	1431.346	34.315	-10.9565
5700	280.419	1401.207	946.504	700.678	1459.385	32.078	-10.9505
5800	280.496	1429.252	951.382	704.959	1487.430	29.784	-10.9467
5900	280.569	1457.305	956.177	709.176	1515.482	27.398	-10.9426
6000	280.638	1485.366	960.893	713.332	1543.543	24.945	-10.9390

TABLE II. - Continued.

II(e) PHENOXY RADICAL (C_6H_5O)

T	C_p°	$H_T^\circ - H_{298.15}^\circ$	S°	$-(G_T^\circ - H_{298.15}^\circ)/T$	H_T°	$\Delta_f H_T^\circ$	$\log_{10} K$
K	J/g-mol K	kJ/g-mol	J/g-mol K	J/g-mol K	kJ/g-mol	kJ/g-mol	
0	-------	-16.208	-------	-------	31.490	63.304	-------
100	39.361	-12.734	242.947	370.289	34.963	57.474	-35.2924
200	63.313	-7.708	276.835	315.378	39.989	52.350	-20.8080
298.15	94.141	-0.000	307.784	307.784	47.698	47.698	-16.4843
300	94.730	0.175	308.368	307.786	47.872	47.609	-16.4321
400	124.786	11.185	339.836	311.872	58.883	43.749	-14.4415
500	149.791	24.959	370.468	320.549	72.657	40.724	-13.3360
600	169.735	40.974	399.611	331.321	88.672	38.372	-12.6484
700	185.681	58.773	427.017	343.055	106.471	36.557	-12.1813
800	198.637	78.011	452.686	355.172	125.708	35.218	-11.8475
900	209.332	98.426	476.719	367.357	146.123	34.268	-11.5936
1000	218.272	119.819	499.251	379.431	167.517	33.692	-11.3963
1100	225.811	142.034	520.418	391.296	189.731	33.403	-11.2380
1200	232.215	164.944	540.348	402.895	212.641	33.334	-11.1063
1300	237.685	188.446	559.157	414.199	236.143	33.433	-10.9943
1400	242.381	212.455	576.947	425.194	260.152	33.695	-10.8976
1500	246.431	236.900	593.811	435.878	284.598	34.037	-10.8136
1600	249.941	261.723	609.830	446.253	309.421	34.489	-10.7395
1700	252.996	286.873	625.077	456.328	334.571	34.951	-10.6723
1800	255.667	312.309	639.615	466.109	360.007	35.456	-10.6126
1900	258.012	337.996	653.502	475.609	385.693	35.980	-10.5581
2000	260.078	363.903	666.790	484.839	411.600	36.468	-10.5087
2100	261.907	390.004	679.524	493.808	437.701	36.955	-10.4623
2200	263.531	416.277	691.746	502.529	463.974	37.408	-10.4199
2300	264.979	442.704	703.493	511.013	490.401	37.830	-10.3822
2400	266.275	469.268	714.799	519.270	516.965	38.179	-10.3458
2500	267.438	495.954	725.692	527.310	543.652	38.516	-10.3125
2600	268.486	522.752	736.202	535.144	570.449	38.755	-10.2813
2700	269.432	549.648	746.353	542.779	597.346	38.944	-10.2527
2800	270.289	576.634	756.167	550.226	624.332	39.064	-10.2249
2900	271.067	603.703	765.666	557.492	651.401	39.129	-10.2005
3000	271.777	630.846	774.868	564.586	678.544	39.106	-10.1770
3100	272.424	658.056	783.790	571.513	705.754	39.028	-10.1550
3200	273.017	685.328	792.448	578.283	733.026	38.839	-10.1337
3300	273.560	712.658	800.858	584.901	760.355	38.607	-10.1149
3400	274.060	740.038	809.032	591.373	787.736	38.255	-10.0967
3500	274.521	767.469	816.983	597.706	815.167	37.853	-10.0802
3600	274.946	794.941	824.722	603.905	842.639	37.357	-10.0647
3700	275.340	822.457	832.261	609.975	870.154	36.769	-10.0497
3800	275.705	850.010	839.609	615.922	897.707	36.110	-10.0370
3900	276.044	877.596	846.775	621.750	925.294	35.334	-10.0234
4000	276.359	905.218	853.768	627.464	952.915	34.484	-10.0124
4100	276.652	932.869	860.596	633.067	980.566	33.540	-10.0021
4200	276.925	960.548	867.266	638.564	1008.245	32.526	-9.9922
4300	277.181	988.252	873.785	643.959	1035.950	31.403	-9.9828
4400	277.420	1015.982	880.160	649.255	1063.680	30.183	-9.9747
4500	277.644	1043.736	886.397	654.456	1091.433	28.877	-9.9666
4600	277.854	1071.510	892.501	659.564	1119.207	27.480	-9.9595
4700	278.052	1099.306	898.479	664.584	1147.004	25.971	-9.9521
4800	278.238	1127.122	904.335	669.518	1174.819	24.393	-9.9460
4900	278.413	1154.954	910.074	674.369	1202.652	22.709	-9.9412
5000	278.578	1182.803	915.700	679.140	1230.501	20.942	-9.9364
5100	278.733	1210.669	921.219	683.833	1258.367	19.069	-9.9325
5200	278.880	1238.550	926.633	688.450	1286.247	17.121	-9.9290
5300	279.019	1266.444	931.946	692.994	1314.142	15.073	-9.9265
5400	279.151	1294.354	937.163	697.468	1342.052	12.917	-9.9238
5500	279.276	1322.275	942.286	701.872	1369.973	10.692	-9.9209
5600	279.394	1350.207	947.319	706.211	1397.905	8.387	-9.9195
5700	279.506	1378.154	952.266	710.484	1425.851	5.983	-9.9179
5800	279.613	1406.109	957.128	714.695	1453.807	3.506	-9.9183
5900	279.714	1434.076	961.908	718.844	1481.773	0.935	-9.9184
6000	279.811	1462.053	966.610	722.935	1509.750	-1.743	-9.9179

TABLE II. - Continued.

II(f) PHENOL (C_6H_5OH)

T	C°_p	$H^\circ_T - H^\circ_{298.15}$	S°	$-(G^\circ_T - H^\circ_{298.15})/T$	H°_T	$\Delta_f H^\circ_T$	$\log_{10} K$
K	J/g-mol K	kJ/g-mol	J/g-mol K	J/g-mol K	kJ/g-mol	kJ/g-mol	
0	-------	-17.496	-------	-------	-113.895	-77.847	-------
100	41.597	-13.972	244.151	383.867	-110.371	-85.126	36.6281
200	69.837	-8.487	281.048	323.483	-104.886	-91.139	13.7709
298.15	103.337	-0.000	315.128	315.128	-96.399	-96.399	5.7340
300	103.968	0.192	315.769	315.130	-96.207	-96.498	5.6306
400	135.869	12.226	350.168	319.604	-84.173	-100.787	1.3392
500	161.960	27.167	383.402	329.067	-69.232	-104.106	-1.3338
600	182.519	44.432	414.822	340.768	-51.967	-106.672	-3.1697
700	198.869	63.531	444.231	353.472	-32.868	-108.656	-4.5075
800	212.165	84.105	471.683	366.552	-12.294	-110.136	-5.5288
900	223.203	105.890	497.329	379.674	9.491	-111.204	-6.3298
1000	232.504	128.688	521.341	392.653	32.289	-111.877	-6.9770
1100	240.423	152.345	543.882	405.387	55.946	-112.242	-7.5102
1200	247.211	176.735	565.100	417.821	80.336	-112.371	-7.9550
1300	253.062	201.756	585.125	429.928	105.357	-112.313	-8.3309
1400	258.127	227.321	604.068	441.696	130.922	-112.077	-8.6526
1500	262.529	253.359	622.031	453.125	156.960	-111.747	-8.9311
1600	266.369	279.808	639.099	464.219	183.409	-111.294	-9.1743
1700	269.732	306.617	655.351	474.988	210.218	-110.821	-9.3871
1800	272.687	333.741	670.853	485.442	237.342	-110.295	-9.5761
1900	275.293	361.142	685.668	495.593	264.743	-109.742	-9.7442
2000	277.601	388.790	699.849	505.454	292.391	-109.218	-9.8951
2100	279.650	416.654	713.443	515.037	320.255	-108.690	-10.0300
2200	281.477	444.712	726.496	524.354	348.313	-108.193	-10.1521
2300	283.111	472.943	739.045	533.417	376.544	-107.722	-10.2646
2400	284.576	501.328	751.125	542.239	404.929	-107.322	-10.3660
2500	285.895	529.853	762.769	550.828	433.454	-106.930	-10.4594
2600	287.085	558.503	774.006	559.197	462.104	-106.638	-10.5451
2700	288.162	587.267	784.861	567.355	490.868	-106.394	-10.6246
2800	289.140	616.132	795.359	575.312	519.733	-106.221	-10.6972
2900	290.029	645.092	805.521	583.075	548.693	-106.102	-10.7662
3000	290.841	674.136	815.367	590.655	577.737	-106.071	-10.8299
3100	291.583	703.257	824.916	598.059	606.858	-106.098	-10.8894
3200	292.262	732.449	834.185	605.294	636.050	-106.238	-10.9445
3300	292.887	761.707	843.188	612.367	665.308	-106.422	-10.9975
3400	293.462	791.024	851.939	619.285	694.625	-106.731	-11.0468
3500	293.992	820.399	860.454	626.054	724.000	-107.092	-11.0939
3600	294.482	849.821	868.743	632.681	753.422	-107.550	-11.1385
3700	294.936	879.293	876.818	639.171	782.894	-108.103	-11.1803
3800	295.357	908.809	884.689	645.529	812.410	-108.734	-11.2214
3900	295.748	938.363	892.366	651.760	841.964	-109.483	-11.2589
4000	296.112	967.958	899.859	657.869	871.559	-110.311	-11.2964
4100	296.451	997.586	907.174	663.861	901.187	-111.238	-11.3321
4200	296.767	1027.248	914.322	669.740	930.849	-112.238	-11.3662
4300	297.063	1056.938	921.308	675.509	960.539	-113.354	-11.3986
4400	297.340	1086.658	928.141	681.173	990.259	-114.572	-11.4305
4500	297.599	1116.406	934.826	686.736	1020.007	-115.881	-11.4606
4600	297.843	1146.177	941.370	692.201	1049.778	-117.285	-11.4900
4700	298.072	1175.973	947.778	697.571	1079.574	-118.809	-11.5176
4800	298.288	1205.793	954.056	702.849	1109.394	-120.404	-11.5450
4900	298.491	1235.631	960.208	708.039	1139.232	-122.112	-11.5724
5000	298.682	1265.490	966.240	713.143	1169.091	-123.907	-11.5985
5100	298.863	1295.367	972.157	718.164	1198.968	-125.814	-11.6242
5200	299.034	1325.262	977.962	723.104	1228.863	-127.800	-11.6492
5300	299.195	1355.173	983.660	727.967	1258.774	-129.890	-11.6743
5400	299.348	1385.102	989.254	732.754	1288.703	-132.095	-11.6980
5500	299.493	1415.043	994.747	737.467	1318.644	-134.370	-11.7206
5600	299.630	1444.998	1000.145	742.110	1348.599	-136.729	-11.7438
5700	299.761	1474.969	1005.450	746.684	1378.570	-139.194	-11.7660
5800	299.885	1504.951	1010.665	751.191	1408.552	-141.731	-11.7893
5900	300.003	1534.946	1015.792	755.631	1438.547	-144.365	-11.8116
6000	300.116	1564.953	1020.835	760.010	1468.554	-147.113	-11.8325

TABLE II. - Continued.

II(g) o-BIPHENYL RADICAL ($C_{12}H_9$)

T	C°_p	$H^\circ_T - H^\circ_{298.15}$	S°	$-(G^\circ_T - H^\circ_{298.15})/T$	H°_T	$\Delta_f H^\circ_T$	$\log_{10} K$
K	J/g-mol K	kJ/g-mol	J/g-mol K	J/g-mol K	kJ/g-mol	kJ/g-mol	
0	-------	-26.589	-------	-------	401.142	451.852	-------
100	63.114	-21.861	294.226	512.833	405.870	442.378	-239.9512
200	109.401	-13.343	351.430	418.147	414.387	434.853	-125.1896
298.15	163.045	-0.000	404.999	404.999	427.730	427.730	-88.0704
300	164.069	0.303	406.011	405.002	428.033	427.587	-87.6069
400	216.776	19.398	460.581	412.086	447.129	421.365	-69.1264
500	261.314	43.379	513.907	427.150	471.109	416.269	-58.1833
600	297.207	71.371	564.844	445.892	499.101	412.152	-50.9732
700	326.066	102.585	612.904	466.353	530.316	408.861	-45.8654
800	349.568	136.406	658.030	487.522	564.136	406.343	-42.0653
900	368.976	172.363	700.358	508.344	600.093	404.461	-39.1205
1000	385.181	210.094	740.098	530.003	637.825	403.219	-36.7764
1100	398.825	249.314	777.467	550.818	677.044	402.459	-34.8656
1200	410.385	289.790	812.679	571.187	717.520	402.065	-33.2744
1300	420.234	331.334	845.926	591.054	759.064	401.949	-31.9279
1400	428.665	373.790	877.386	610.393	801.520	402.104	-30.7733
1500	435.916	417.027	907.214	629.196	844.757	402.382	-29.7731
1600	442.180	460.940	935.552	647.465	888.670	402.845	-28.8980
1700	447.616	505.436	962.526	665.211	933.166	403.302	-28.1227
1800	452.354	550.440	988.248	682.448	978.171	403.828	-27.4346
1900	456.501	595.887	1012.819	699.194	1023.618	404.376	-26.8175
2000	460.145	641.724	1036.330	715.468	1069.454	404.842	-26.2621
2100	463.361	687.902	1058.859	731.287	1115.632	405.299	-25.7569
2200	466.209	734.383	1080.482	746.671	1162.113	405.688	-25.2977
2300	468.742	781.133	1101.263	761.640	1208.863	406.014	-24.8810
2400	471.002	828.122	1121.261	776.210	1255.852	406.196	-24.4957
2500	473.027	875.326	1140.530	790.400	1303.056	406.361	-24.1422
2600	474.845	922.721	1159.119	804.226	1350.451	406.334	-23.8155
2700	476.484	970.289	1177.071	817.705	1398.019	406.216	-23.5137
2800	477.965	1018.013	1194.427	830.851	1445.743	405.972	-23.2316
2900	479.308	1065.877	1211.223	843.679	1493.607	405.623	-22.9719
3000	480.528	1113.869	1227.493	856.203	1541.599	405.107	-22.7285
3100	481.641	1161.978	1243.267	868.436	1589.708	404.495	-22.5010
3200	482.658	1210.196	1258.577	880.391	1637.926	403.678	-22.2867
3300	483.589	1258.509	1273.443	892.076	1686.240	402.781	-22.0880
3400	484.443	1306.910	1287.892	903.507	1734.641	401.657	-21.9002
3500	485.229	1355.394	1301.946	914.691	1783.124	400.440	-21.7243
3600	485.954	1403.954	1315.626	925.639	1831.685	399.055	-21.5590
3700	486.623	1452.582	1328.950	936.360	1880.312	397.494	-21.4018
3800	487.242	1501.276	1341.936	946.863	1929.006	395.803	-21.2561
3900	487.817	1550.031	1354.600	957.156	1977.761	393.898	-21.1150
4000	488.350	1598.840	1366.958	967.248	2026.570	391.851	-20.9846
4100	488.846	1647.697	1379.022	977.144	2075.428	389.628	-20.8612
4200	489.308	1696.606	1390.808	986.854	2124.337	387.280	-20.7437
4300	489.740	1745.560	1402.326	996.382	2173.290	384.732	-20.6318
4400	490.143	1794.553	1413.590	1005.737	2222.284	381.999	-20.5267
4500	490.520	1843.586	1424.609	1014.924	2271.317	379.109	-20.4258
4600	490.874	1892.659	1435.394	1023.947	2320.389	376.053	-20.3304
4700	491.206	1941.761	1445.954	1032.813	2369.492	372.782	-20.2381
4800	491.518	1990.898	1456.300	1041.530	2418.628	369.387	-20.1517
4900	491.811	2040.065	1466.438	1050.098	2467.795	365.797	-20.0710
5000	492.087	2089.261	1476.377	1058.525	2516.992	362.061	-19.9931
5100	492.347	2138.481	1486.124	1066.814	2566.212	358.123	-19.9196
5200	492.593	2187.729	1495.687	1074.970	2615.459	354.055	-19.8496
5300	492.826	2237.000	1505.072	1082.997	2664.730	349.803	-19.7840
5400	493.045	2286.292	1514.285	1090.898	2714.022	345.347	-19.7204
5500	493.253	2335.609	1523.335	1098.679	2763.339	340.777	-19.6582
5600	493.450	2384.944	1532.224	1106.341	2812.674	336.069	-19.6013
5700	493.637	2434.297	1540.960	1113.891	2862.027	331.172	-19.5460
5800	493.815	2483.671	1549.547	1121.328	2911.402	326.157	-19.4963
5900	493.983	2533.060	1557.989	1128.657	2960.790	320.970	-19.4478
6000	494.144	2582.468	1566.294	1135.882	3010.198	315.592	-19.3998

TABLE II. - Continued.

II(h) BIPHENYL ($C_{12}H_{10}$)

T	C°_p	$H^\circ_T - H^\circ_{298.15}$	S°	$-(G^\circ_T - H^\circ_{298.15})/T$	H°_f	$\Delta_f H^\circ_f$	$\log_{10} K$
K	J/g-mol K	kJ/g-mol	J/g-mol K	J/g-mol K	kJ/g-mol	kJ/g-mol	
0	-------	-26.783	-------	-------	155.347	210.292	-------
100	83.120	-22.053	277.279	497.807	160.077	199.319	-116.5054
200	110.045	-13.517	334.587	402.173	168.613	190.466	-65.3587
298.15	166.175	-0.000	388.830	388.330	182.130	182.130	-49.2975
300	167.255	0.308	389.861	388.833	182.438	181.966	-49.0993
400	222.983	19.876	445.768	396.078	202.006	174.764	-41.3307
500	270.062	44.609	500.763	411.545	226.739	168.957	-36.8372
600	307.965	73.580	553.479	430.845	255.710	164.356	-33.9373
700	338.456	105.955	603.324	451.960	288.085	160.756	-31.9133
800	363.331	141.084	650.196	473.841	323.214	158.070	-30.4283
900	383.924	178.478	694.216	495.907	360.608	156.138	-29.2848
1000	401.165	217.758	735.586	517.828	399.888	154.941	-28.3818
1100	415.718	258.622	774.522	539.411	440.752	154.307	-27.6497
1200	428.077	300.828	811.238	560.548	482.958	154.104	-27.0402
1300	438.629	344.178	845.930	581.178	526.308	154.232	-26.5236
1400	447.678	388.504	878.776	601.273	570.634	154.676	-26.0795
1500	455.473	433.671	909.935	620.821	615.801	155.279	-25.6943
1600	462.218	479.564	939.551	639.824	661.694	156.097	-25.3566
1700	468.078	526.086	967.753	658.291	708.216	156.933	-25.0549
1800	473.192	573.155	994.656	676.236	755.285	157.856	-24.7870
1900	477.672	620.703	1020.363	693.677	802.833	158.819	-24.5452
2000	481.614	668.671	1044.966	710.631	850.801	159.713	-24.3270
2100	485.095	717.010	1068.550	727.117	899.140	160.608	-24.1265
2200	488.181	765.676	1091.189	743.154	947.806	161.442	-23.9436
2300	490.928	814.635	1112.952	758.763	996.765	162.222	-23.7788
2400	493.381	863.853	1133.898	773.960	1045.983	162.863	-23.6241
2500	495.578	913.302	1154.084	788.763	1095.432	163.488	-23.4822
2600	497.554	962.961	1173.560	803.191	1145.091	163.926	-23.3505
2700	499.335	1012.807	1192.373	817.259	1194.937	164.274	-23.2289
2800	500.947	1062.822	1210.562	830.983	1244.952	164.495	-23.1137
2900	502.408	1112.991	1228.167	844.377	1295.121	164.615	-23.0093
3000	503.737	1163.299	1245.222	857.456	1345.429	164.567	-22.9104
3100	504.948	1213.733	1261.759	870.232	1395.863	164.420	-22.8179
3200	506.057	1264.286	1277.810	882.720	1446.416	164.066	-22.7299
3300	507.072	1314.944	1293.397	894.929	1497.074	163.632	-22.6496
3400	508.004	1365.698	1308.549	906.873	1547.828	162.969	-22.5730
3500	508.861	1416.541	1323.287	918.561	1598.671	162.210	-22.5018
3600	509.652	1467.468	1337.633	930.004	1649.598	161.279	-22.4351
3700	510.383	1518.468	1351.607	941.210	1700.598	160.167	-22.3711
3800	511.059	1569.542	1365.228	952.190	1751.672	158.924	-22.3134
3900	511.687	1620.681	1378.511	962.952	1802.811	157.460	-22.2558
4000	512.270	1671.879	1391.473	973.504	1854.009	155.852	-22.2045
4100	512.812	1723.131	1404.129	983.853	1905.261	154.062	-22.1562
4200	513.318	1774.439	1416.493	994.007	1956.569	152.145	-22.1101
4300	513.789	1825.795	1428.577	1003.974	2007.925	150.020	-22.0661
4400	514.230	1877.195	1440.394	1013.759	2059.325	147.706	-22.0257
4500	514.643	1928.639	1451.955	1023.369	2110.769	145.229	-21.9866
4600	515.031	1980.125	1463.271	1032.809	2162.255	142.583	-21.9502
4700	515.394	2031.645	1474.350	1042.085	2213.775	139.714	-21.9143
4800	515.735	2083.202	1485.206	1051.205	2265.332	136.719	-21.8817
4900	516.056	2134.792	1495.843	1060.171	2316.922	133.523	-21.8526
5000	516.359	2186.415	1506.273	1068.989	2368.545	130.176	-21.8243
5100	516.644	2238.063	1516.500	1077.664	2420.193	126.619	-21.7982
5200	516.914	2289.741	1526.535	1086.200	2471.871	122.930	-21.7738
5300	517.163	2341.445	1536.384	1094.602	2523.575	119.053	-21.7520
5400	517.409	2393.174	1546.053	1102.872	2575.304	114.966	-21.7304
5500	517.637	2444.928	1555.549	1111.017	2627.058	110.763	-21.7088
5600	517.853	2496.703	1564.878	1119.038	2678.833	106.416	-21.6908
5700	518.058	2548.496	1574.046	1126.941	2730.626	101.877	-21.6731
5800	518.253	2600.314	1583.058	1134.728	2782.444	97.217	-21.6596
5900	518.438	2652.145	1591.918	1142.402	2834.275	92.381	-21.6460
6000	518.614	2704.000	1600.633	1149.967	2886.130	87.353	-21.6316

TABLE II. - Continued.

II(i) o-BIPHENYL-d_9 ($C_{12}D_9$)

T	C°_p	$H^\circ_T - H^\circ_{298.15}$	S°	$-(G^\circ_T - H^\circ_{298.15})/T$	H°_T	$\Delta_f H^\circ_T$	$\log_{10} K$
K	J/g-mol K	kJ/g-mol	J/g-mol K	J/g-mol K	kJ/g-mol	kJ/g-mol	
0	-------	-30.602	-------	-------	355.905	407.068	-------
100	68.275	-25.702	299.472	556.494	360.805	398.895	-219.7996
200	129.644	-15.968	364.505	444.344	370.539	391.420	-116.4292
298.15	194.584	-0.000	428.598	428.598	386.507	386.507	-82.9723
300	195.724	0.361	429.805	428.602	386.868	386.423	-82.5533
400	251.054	22.803	493.984	436.977	409.310	383.471	-65.8016
500	294.984	50.190	554.915	454.535	436.697	381.763	-55.8079
600	329.861	81.498	611.900	476.069	468.005	380.868	-49.1719
700	357.726	115.929	664.919	499.307	502.436	380.604	-44.4349
800	380.102	152.860	714.201	523.126	539.367	380.878	-40.8862
900	398.154	191.805	760.050	546.934	578.312	381.513	-38.1168
1000	412.792	232.377	802.784	570.406	618.884	382.527	-35.8999
1100	424.734	274.274	842.706	593.367	660.781	383.748	-34.0824
1200	434.542	317.253	880.097	615.720	703.761	385.105	-32.5620
1300	442.656	361.126	915.210	637.421	747.633	386.488	-31.2696
1400	449.417	405.739	948.269	658.455	792.246	387.954	-30.1572
1500	455.092	450.973	979.475	678.827	837.480	389.362	-29.1910
1600	459.890	496.729	1009.004	698.548	883.236	390.821	-28.3441
1700	463.973	542.927	1037.010	717.641	929.434	392.133	-27.5898
1800	467.471	589.504	1063.632	736.130	976.011	393.403	-26.9209
1900	470.486	636.405	1088.990	754.040	1022.913	394.595	-26.3190
2000	473.101	683.588	1113.190	771.396	1070.095	395.636	-25.7766
2100	475.381	731.015	1136.329	788.227	1117.522	396.569	-25.2816
2200	477.378	778.654	1158.491	804.558	1165.161	397.421	-24.8337
2300	479.138	826.483	1179.751	820.411	1212.990	398.129	-24.4249
2400	480.694	874.474	1200.177	835.812	1260.982	398.654	-24.0460
2500	482.077	922.615	1219.828	850.782	1309.122	399.134	-23.6994
2600	483.312	970.887	1238.761	865.343	1357.394	399.382	-23.3779
2700	484.416	1019.273	1257.022	879.513	1405.780	399.517	-23.0818
2800	485.409	1067.765	1274.657	893.313	1454.272	399.514	-22.8041
2900	486.305	1116.352	1291.707	906.758	1502.859	399.360	-22.5487
3000	487.116	1165.024	1308.207	919.866	1551.531	399.016	-22.3088
3100	487.852	1213.773	1324.192	932.652	1600.280	398.573	-22.0845
3200	488.521	1262.592	1339.692	945.132	1649.099	397.924	-21.8740
3300	489.132	1311.475	1354.733	957.317	1697.982	397.163	-21.6770
3400	489.691	1360.417	1369.345	969.222	1746.924	396.185	-21.4925
3500	490.204	1409.412	1383.547	980.858	1795.919	395.085	-21.3179
3600	490.674	1458.455	1397.363	992.236	1844.962	393.825	-21.1554
3700	491.109	1507.547	1410.813	1003.368	1894.055	392.370	-21.0001
3800	491.509	1556.675	1423.915	1014.264	1943.182	390.793	-20.8567
3900	491.880	1605.846	1436.687	1024.932	1992.354	388.984	-20.7180
4000	492.224	1655.052	1449.145	1035.382	2041.559	387.033	-20.5882
4100	492.543	1704.290	1461.303	1045.623	2090.797	384.907	-20.4666
4200	492.839	1753.559	1473.176	1055.662	2140.066	382.656	-20.3501
4300	493.116	1802.858	1484.777	1065.507	2189.365	380.190	-20.2402
4400	493.375	1852.185	1496.116	1075.165	2238.692	377.563	-20.1356
4500	493.615	1901.531	1507.207	1084.644	2288.039	374.762	-20.0362
4600	493.841	1950.904	1518.057	1093.948	2337.411	371.799	-19.9424
4700	494.052	2000.300	1528.681	1103.085	2386.807	368.632	-19.8510
4800	494.251	2049.716	1539.085	1112.061	2436.223	365.329	-19.7655
4900	494.437	2099.150	1549.277	1120.879	2485.657	361.837	-19.6858
5000	494.613	2148.602	1559.269	1129.549	2535.109	358.224	-19.6083
5100	494.778	2198.073	1569.065	1138.070	2584.580	354.405	-19.5352
5200	494.934	2247.559	1578.674	1146.452	2634.066	350.463	-19.4667
5300	495.081	2297.060	1588.103	1154.696	2683.567	346.329	-19.4017
5400	495.220	2346.575	1597.359	1162.808	2733.082	342.020	-19.3389
5500	495.352	2396.103	1606.447	1170.792	2782.610	337.587	-19.2766
5600	495.476	2445.644	1615.374	1178.652	2832.151	333.027	-19.2207
5700	495.594	2495.196	1624.144	1186.391	2881.704	328.292	-19.1656
5800	495.706	2544.760	1632.764	1194.012	2931.268	323.448	-19.1161
5900	495.813	2594.338	1641.239	1201.521	2980.845	318.430	-19.0678
6000	495.914	2643.924	1649.573	1208.919	3030.431	313.270	-19.0215

TABLE II. - Concluded.

II(j) BIPHENYL-d_{10} ($C_{12}D_{10}$)

T	C°_p	$H^\circ_T - H^\circ_{298.15}$	S°	$-(G^\circ_T - H^\circ_{298.15})/T$	H°_T	$\Delta_f H^\circ_T$	$\log_{10} K$
K	J/g-mol K	kJ/g-mol	J/g-mol K	J/g-mol K	kJ/g-mol	kJ/g-mol	
0	-------	-30.941	-------	-------	107.473	162.920	-------
100	68.295	-26.038	282.781	543.163	112.376	153.375	-95.3701
200	131.011	-16.258	348.082	429.372	122.156	144.470	-56.2700
298.15	199.254	-0.000	413.311	413.311	138.414	138.414	-44.0896
300	200.459	0.370	414.548	413.315	138.784	138.311	-43.9386
400	259.062	23.454	480.551	421.917	161.868	134.542	-38.0042
500	305.628	51.778	543.563	440.006	190.193	132.306	-34.5186
600	342.628	84.261	602.683	462.248	222.675	131.111	-32.2288
700	372.238	120.058	657.806	486.295	258.472	130.725	-30.5988
800	396.060	158.516	709.123	510.979	296.930	131.011	-29.3809
900	415.314	199.118	756.923	535.681	337.532	131.764	-28.4238
1000	430.955	241.458	801.518	560.060	379.872	132.979	-27.6558
1100	443.735	285.214	843.213	583.928	423.628	134.464	-27.0227
1200	454.247	330.130	882.288	607.180	468.544	136.134	-26.4883
1300	462.954	376.003	919.002	629.769	514.417	137.865	-26.0289
1400	470.218	422.672	953.584	651.676	561.086	139.710	-25.6295
1500	476.322	470.008	986.240	672.902	608.422	141.519	-25.2803
1600	481.489	517.906	1017.151	693.460	656.320	143.401	-24.9724
1700	485.890	566.280	1046.477	713.371	704.695	145.143	-24.6928
1800	489.664	615.063	1074.359	732.658	753.477	146.865	-24.4452
1900	492.921	664.196	1100.924	751.347	802.610	148.513	-24.2195
2000	495.747	713.633	1126.280	769.464	852.047	150.017	-24.0150
2100	498.213	763.334	1150.529	787.036	901.748	151.417	-23.8251
2200	500.376	813.265	1173.757	804.091	951.679	152.742	-23.6542
2300	502.282	863.400	1196.043	820.651	1001.814	153.924	-23.4977
2400	503.969	913.713	1217.456	836.742	1052.128	154.928	-23.3497
2500	505.470	964.188	1238.060	852.385	1102.602	155.888	-23.2151
2600	506.811	1014.804	1257.912	867.603	1153.218	156.614	-23.0888
2700	508.011	1065.545	1277.062	882.415	1203.959	157.230	-22.9733
2800	509.090	1116.401	1295.557	896.842	1254.815	157.705	-22.8627
2900	510.065	1167.360	1313.439	910.901	1305.774	158.029	-22.7627
3000	510.947	1218.411	1330.746	924.609	1356.825	158.160	-22.6676
3100	511.748	1269.547	1347.513	937.982	1407.961	158.192	-22.5784
3200	512.477	1320.758	1363.773	951.036	1459.172	158.015	-22.4944
3300	513.142	1372.040	1379.553	963.783	1510.454	157.724	-22.4159
3400	513.752	1423.386	1394.882	976.239	1561.800	157.212	-22.3428
3500	514.311	1474.789	1409.782	988.414	1613.203	156.574	-22.2729
3600	514.825	1526.245	1424.277	1000.320	1664.659	155.776	-22.2092
3700	515.300	1577.754	1438.390	1011.970	1716.168	154.775	-22.1471
3800	515.736	1629.302	1452.138	1023.374	1767.717	153.650	-22.0919
3900	516.142	1680.899	1465.539	1034.540	1819.313	152.289	-22.0368
4000	516.517	1732.531	1478.612	1045.479	1870.946	150.780	-21.9861
4100	516.866	1784.201	1491.370	1056.200	1922.615	149.094	-21.9397
4200	517.190	1835.904	1503.830	1066.710	1974.318	147.279	-21.8947
4300	517.493	1887.639	1516.003	1077.018	2026.053	145.240	-21.8528
4400	517.776	1939.404	1527.904	1087.130	2077.819	143.041	-21.8130
4500	518.039	1991.193	1539.543	1097.056	2129.607	140.658	-21.7754
4600	518.286	2043.008	1550.931	1106.798	2181.423	138.110	-21.7407
4700	518.518	2094.850	1562.080	1116.367	2233.264	135.355	-21.7057
4800	518.735	2146.713	1572.999	1125.767	2285.127	132.456	-21.6741
4900	518.939	2198.597	1583.697	1135.004	2337.011	129.365	-21.6461
5000	519.131	2250.499	1594.184	1144.084	2388.913	126.151	-21.6181
5100	519.312	2302.423	1604.465	1153.010	2440.837	122.724	-21.5925
5200	519.484	2354.364	1614.551	1161.789	2492.778	119.172	-21.5697
5300	519.645	2406.320	1624.448	1170.425	2544.734	115.421	-21.5485
5400	519.797	2458.292	1634.163	1178.923	2596.706	111.494	-21.5277
5500	519.941	2510.279	1643.702	1187.287	2648.693	107.441	-21.5059
5600	520.078	2562.279	1653.072	1195.522	2700.694	103.257	-21.4890
5700	520.207	2614.292	1662.278	1203.630	2752.706	98.894	-21.4714
5800	520.330	2666.318	1671.326	1211.616	2804.732	94.423	-21.4582
5900	520.447	2718.359	1680.222	1219.483	2856.773	89.774	-21.4448
6000	520.558	2770.408	1688.970	1227.235	2908.822	84.982	-21.4323

TABLE III. - COMPARISON OF RESULTS FROM DIFFERENT CALCULATIONS[a]

Property	Bahn[b]	Benson	From benzene[c]	From phenol[c]
Phenyl radical				
$S°_{300}$	71.73	69.4[d]	69.03	69.30
$C°_{p300}$	23.57	18.8	18.96	19.51
$C°_{p500}$	32.44	-----	31.03	31.70
$C°_{p1000}$	45.93	-----	46.59	46.93
$C°_{p3000}$	58.44	-----	59.04	59.09
Phenoxy radical				
$S°_{300}$	-----	73.7[e]	-----	73.70
$C°_{p300}$	-----	22.5	-----	22.64
$C°_{p400}$	-----	29.8	-----	29.82
$C°_{p500}$	-----	35.8	-----	35.80
$C°_{p600}$	-----	40.6	-----	40.57
$C°_{p800}$	-----	47.5	-----	47.48
$C°_{p1000}$	-----	52.3	-----	52.17

[a]All values as eu (cal/g-mol k).
[b]From reference 2.
[c]Current calculations.
[d]From reference 4.
[e]From reference 17.

TABLE IV. - COEFFICIENTS FOR NASA TYPE POLYNOMIALS

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C6H5              L12/84C   6H   5    0    0G   300.000  5000.000     77.10550 1
 0.11431418E 02 0.17019045E-01-0.58387241E-05 0.88094687E-09-0.48050417E-13    2
 0.33942348E 05-0.38574219E 02-0.23405075E 01 0.42760305E-01-0.25518166E-05    3
-0.30668716E-07 0.16245519E-10 0.38376734E 05 0.35617355E 02 0.39502977E 05    4

C6H6              L12/84C   6H   6    0    0G   300.000  5000.000     78.11340 1
 0.11815166E 02 0.19169778E-01-0.65425238E-05 0.98228425E-09-0.53280361E-13    2
 0.40707441E 04-0.43973511E 02-0.32181215E 01 0.47168836E-01-0.21254918E-05    3
-0.34879005E-07 0.18425386E-10 0.89017773E 04 0.36999313E 02 0.99586128E 04    4

C6D5              L12/84C   6D   5    0    0G   300.000  5000.000     82.13651 1
 0.14729492E 02 0.15210535E-01-0.55241635E-05 0.87984575E-09-0.50979217E-13    2
 0.30282629E 05-0.55768127E 02-0.12549782E 01 0.47328766E-01-0.80759883E-05    3
-0.29901972E-07 0.17149060E-10 0.35314063E 05 0.29766983E 02 0.36917128E 05    4

C6D6              L12/84C   6D   6    0    0G   300.000  5000.000     84.15061 1
 0.15619864E 02 0.17123934E-01-0.62012759E-05 0.98493058E-09-0.56891557E-13    2
-0.14433052E 03-0.63901352E 02-0.20701218E 01 0.52938197E-01-0.96074828E-05    3
-0.32802372E-07 0.19012528E-10 0.54068984E 04 0.30680710E 02 0.69971633E 04    4

C6H5O             L12/84C   6H   5O   1    0G   300.000  5000.000     93.10490 1
 0.13833984E 02 0.17618403E-01-0.60696257E-05 0.91988173E-09-0.50449181E-13    2
-0.69212549E 03-0.50392990E 02-0.18219433E 01 0.48122510E-01-0.46792302E-05    3
-0.34018594E-07 0.18649637E-10 0.42429180E 04 0.33526199E 02 0.57367379E 04    4

C6H5OH            L12/84C   6H   6O   1    0G   300.000  5000.000     94.11280 1
 0.14930705E 02 0.18346462E-01-0.61796381E-05 0.91533114E-09-0.48830826E-13    2
-0.18379656E 05-0.55983917E 02-0.16495714E 01 0.52105546E-01-0.69632842E-05    3
-0.36011539E-07 0.20483074E-10-0.13292336E 05 0.32357330E 02-0.11594207E 05    4

C12H9             L12/84C  12H   9    0    0G   300.000  5000.000    153.20310 1
 0.23851303E 02 0.31960227E-01-0.11076719E-04 0.16847825E-08-0.92641173E-13    2
 0.40171297E 05-0.10270549E 03-0.31376228E 01 0.82217276E-01-0.40171444E-05    3
-0.60809782E-07 0.32074402E-10 0.48868754E 05 0.42730362E 02 0.51444448E 05    4

C12H10            L12/84C  12H  10    0    0G   300.000  5000.000    154.21100 1
 0.24289017E 02 0.34006648E-01-0.11722408E-04 0.17729298E-08-0.96812532E-13    2
 0.10287000E 05-0.10802374E 03-0.40739527E 01 0.86973310E-01-0.42353613E-05    3
-0.64564460E-07 0.34150169E-10 0.19405965E 05 0.44741348E 02 0.21905340E 05    4

C12D9             L12/84C  12D   9    0    0G   300.000  5000.000    162.25892 1
 0.30123199E 02 0.28328255E-01-0.10366540E-04 0.16593338E-08-0.96527116E-13    2
 0.33207789E 05-0.13520447E 03-0.73299396E 00 0.89836895E-01-0.13731275E-04    3
-0.59427020E-07 0.33702430E-10 0.42943094E 05 0.30028793E 02 0.46486410E 05    4

C12D10            L12/84C  12D  10    0    0G   300.000  5000.000    164.27302 1
 0.30905060E 02 0.30349988E-01-0.11095048E-04 0.17755810E-08-0.10332327E-12    2
 0.28034453E 04-0.14245210E 03-0.15793486E 01 0.95059574E-01-0.14532071E-04    3
-0.62645597E-07 0.35530079E-10 0.13137422E 05 0.31516678E 02 0.16647502E 05    4
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16. Abstract

Ideal gas thermodynamic properties of the phenyl and o-biphenyl radicals, their deuterated analogs and the phenoxy radical were calculated to 5000 K using estimated vibrational frequencies and structures. The ideal gas thermodynamic properties of benzene, biphenyl, their deuterated analogs and phenol were also calculated.

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