HEAT OF FORMATION (ΔH_f^0) OF HYDROCARBONS AND RELATED COMPOUNDS AT DIFFERENT TEMPERATURES

By T. R. Das, S. H. Ibrahim and N. R. Kuloor

(Department of Chemical Engineering, Indian Institute of Science, Bangalore-12, India)

[Received: April 4, 1968]

Abstract

Based on the use of Molecular weight alone a method of correlating ΔH_f^0 is proposed which predicts the data with an average difference of 0.34 K. cals/g.mole.

The knowledge of heat of reaction is essential in reaction engineering calculations. This heat of reaction can be calculated using standard heat of formation (ΔH_f^0), heat of combustion and heats of other reactions which involve the same compounds. More often the heat of combustion data are frequently available when compared to the heat of formation data. Although it is possible to calculate heat of formation from heat of combustion indirectly, many methods are available to correlate heat of formation.

Reid and Sherwood[1] consider five methods to calculate the standard heat of formation. These methods are due to Souders-Mathews-Hurd (SMH), Franklin, Andersen-Beyer-Watson, Verma-Doraiswamy and Hardrick. All of them use bond energies or additive atomic groups or indirect heat of combustion data. Extensive tabulation of these energies or groups are required in addition to the difficulties involved in calculation of ΔH_f^0 at different temperatures. For hydrocarbons and related compounds SMH method is the best giving an average difference ($\Delta H_{f\,\text{calc.}}^0 - \Delta H_{f\,\text{expl.}}^0$) of 0.5 kcals/g mole, whereas other methods give an average difference of about 3-5 kcals/g mole.

It is desirable to have a method of correlating ΔH_f^0 by using fewer input data and at the same time retaining the high standard of accuracy of the SMH method. The present proposed method to calculate ΔH_f^0 achieves this, using molecular weight as the only input datum, with an average difference of 0.34 kcals/g.mole.

The method used in this work is exactly similar to the one we have used earlier to predict the latent heat of vaporization at its boiling point[2], the

thermal conductivity of organic liquids[3], liquid viscosity[4], liquid heat capacity[5], liquid surface tension[6], normal boiling point[7], liquid kinematic viscosity[7] and the free energy of formation[8]

Detailed experimental data of ΔH_f^0 for hydrocarbons and related compounds are available for temperature range of $0 - 1500\,^{\circ}K$ in API Project 44[9]. By considering six homologs containing 109 compounds and 1635 temperature points we have found that ΔH_f^0 varied linearly with molecular weight when plotted in ordinary co-ordinates for one temperature. The same pattern of linear relationship was observed for all the temperatures between $0 - 1500\,^{\circ}K$. These slopes and intercepts when plotted against temperature gave 3 straight lines for each homolog indicating 3 temperature bands between $300 - 1500\,^{\circ}K$. Because of lack of data between 0 and 298 or $300\,^{\circ}K$, no relationship is possible for this band, but an equation was obtained for $0\,^{\circ}K$, alone. The other temperature bands are: (i) 300 to $500\,^{\circ}K$, (ii) $500 - 1000\,^{\circ}K$ and (iii) 1000 to $1500\,^{\circ}K$. Substituting these slopes and intercepts in the earlier equations between M and ΔH_f^0, a set of 18 equations has been extracted for the six homologs for these three bands. Another 6 more equations have also been added for $0\,^{\circ}K$ because these data may be required to calculate the heat content or the thermodynamic function $(\Delta H_f^0 - \Delta H_{f_0}^0)$. All these 24 equations are shown in Table 1.

These equations have been tested for one representative temperature for each band, namely at $0\,^{\circ}K$, $400\,^{\circ}K$ $800\,^{\circ}K$ and $1200\,^{\circ}K$ and for each homolog and these values are shown in Table 2 for normal paraffins, Table 3 for monoolefins, Table 4 for alkyl benzenes, Table 5 for cyclopentanes, Table 6 for cyclohexanes and Table 7 for normal acetylenes.

Tables 2 to 7 show that the accuracy of these equations in predicting ΔH_f^0 at different temperatures is very good. The first member, as a rule deviates for this types of correlation for all the properties and hence these are excluded from average. The over-all average difference for all the points tested is 0.34 kcals /g.mole.

Nomenclature:

ΔH_f^0 = Standard heat of formation at different temperatures, kcals./g.mole.

$\Delta H_{f_0}^0$ = Standard heat of formation at $0\,^{\circ}K$, kcals./g.mole.

TABLE I

Equations for heat of formation at different temperature for hydrocarbons and related compounds

Series	Temperature range, K	Equation
I. *n* Paraffins	At 0°	$\Delta H^{\circ}_f = M(-0.300 \times 10^{-3}T - 0.2590) - 3.0777 \times 10^{-3}T - 8.9307$
	300 – 500	$\Delta H^{\circ}_f = M(-0.193 \times 10^{-3}T - 0.2963) - 3.9100 \times 10^{-3}T - 8.7200$
	500 – 1000	$\Delta H^{\circ}_f = M(-0.0526 \times 10^{-3}T - 0.3806) - 4.375 \times 10^{-3}T - 8.1625$
	1000 – 1500	$\Delta H^{\circ} = M(0.0333 \times 10^{-3}T - 0.4659) \quad 0.6944 \times 10^{-3}T - 41.7390$
II. Monoolefins	At 0°	$\Delta H^{\circ}_f = M(-0.2907 \times 10^{-3}T - 0.2630) - 2.0830 \times 10^{-3}T + 19.8960$
	300 – 500	$\Delta H^{\circ}_f = M(-0.2110 \times 10^{-3}T - 0.2900) - 2.5960 \times 10^{-3}T + 20.5040$
	500 – 1000	$\Delta H^{\circ}_f = M(-0.0698 \times 10^{-3}T - 0.3644) - 0.8210 \times 10^{-3}T + 19.1367$
	1000 – 1500	$\Delta H^{\circ}_f = M(0.0426 \times 10^{-3}T - 0.4777) - 2.6530 \times 10^{-3}T + 20.7900$
III. Alkylbenzens	At 0°	$\Delta H^{\circ}_f = M(-0.2885 \times 10^{-3}T - 0.2684) + 9.8684 \times 10^{-3}T + 42.1080$
	300 – 500	$\Delta H^{\circ}_f = M(-0.2167 \times 10^{-3}T - 0.2910) + 7.1730 \times 10^{-3}T + 42.1000$
	500 – 1000	$\Delta H^{\circ}_f = M(-0.0540 \times 10^{-3}T - 0.3790) - 0.8333 \times 10^{-3}T + 45.9500$
	1000 – 1500	$\Delta H^{\circ}_f = M(0.0465 \times 10^{-3}T - 0.4832) - 4.1892 \times 10^{-3}T + 49.4838$

TABLE 2—(*concld*)

Series	Temperature range, °K	Equation
IV. Cyclopentanes	At 0°	$\Delta H^\circ_f = M(-0.1951 \times 10^{-3}T - 0.2611) - 4.8750 \times 10^{-3}T + 5.2438$
	300 – 500	$\Delta H^\circ_f = M(-0.2033 \times 10^{-3}T - 0.2934) - 7.0650 \times 10^{-3}T + 6.2770$
	500 – 1000	$\Delta H^\circ_f = M(-0.0550 \times 10^{-3}T - 0.3756) - 2.2435 \times 10^{-3}T + 3.6249$
	1000 – 1500	$\Delta H^\circ_f = M(0.0250 \times 10^{-3}T - 0.4533) - 0.8475 \times 10^{-3}T + 0.4398$
V. Cyclohexanes	At 0°	$\Delta H^\circ_f = M(-0.2830 \times 10^{-3}T - 0.2630) - 6.3414 \times 10^{-3}T + 0.6207$
	300 – 500	$\Delta H^\circ_f = M(-0.1776 \times 10^{-3}T - 0.3005) - 4.4310 \times 10^{-3}T - 0.5570$
	500 – 1000	$\Delta H^\circ_f = M(0.0555 \times 10^{-3}T - 0.3762) + 0.3704 \times 10^{-3}T - 2.5037$
	1000 – 1500	$\Delta H^\circ_f = M(0.0349 \times 10^{-3}T - 0.4648) + 3.9062 \times 10^{-3}T - 6.2702$
VI. *n*-Acetylenes	At 0°	$\Delta H^\circ_f = M(-0.2973 \times 10^{-3}T - 0.2591) + 6.1224 \times 10^{-3}T + 56.4102$
	300 – 500	$\Delta H^\circ_f = M(-0.2066 \times 10^{-3}T - 0.2910) + 4.9990 \times 10^{-3}T + 56.5510$
	500 – 1000	$\Delta H^\circ_f = M(-0.0617 \times 10^{-3}T - 0.3733) - 1.6900 \times 10^{-3}T + 60.5700$
	1000 – 1500	$\Delta H^\circ_f = M(0.0523 \times 10^{-3}T - 0.4916) - 3.9773 \times 10^{-3}T + 63.3470$

TAB
Heat of formation ($-H°_f$) of normal

n-Paraffins	Mol. wt.	API Proj. 44	0°K Calc.	Diff.	API Proj. 44	400°K Calc.
Methane	16.0	– 15 99	– 13.07	2 92	– 18 63	– 16.26
Ethane	30.0	– 16 52	– 16.70	– 0.18	– 21.42	– 21.48
Propane	44 0	– 19.48	– 20.33	– 0 85	– 26.36	– 26 71
n-Butane	58.1	– 23 67	– 23.98	– 0.31	– 32.00	– 31.98
n-Pentane	72.1	– 27.23	– 27.60	– 0.37	– 37.18	– 37.21
n-Heptane	86.2	– 30 91	– 31.25	– 0.34	– 42.46	– 42.47
n-Hexane	100.2	– 34 55	– 34.88	– 0 33	– 47.71	– 47.70
n-Octane	114.2	– 38.20	– 38.51	– 0.31	– 52 96	– 52.93
n-Nonane	128.3	– 41.84	– 42.16	– 0 32	– 58.22	– 58 20
n-Decane	142.3	– 45.49	– 45.78	– 0 29	– 63.47	– 63 43
n-Undecane	156.3	– 49.13	– 49.41	– 0.28	– 68.72	– 68.66
n-Dodecane	170 3	– 52 77	– 53.04	– 0.27	– 73.97	– 73.89
n-Tridecane	184 4	– 56.42	– 56.69	– 0.27	– 79.22	– 79.15
n-Tetradecane	198.4	– 60 06	– 60.31	– 0 25	– 84.48	– 84 38
n-Pentadecane	212 4	– 63.71	– 63.94	– 0.23	– 89.73	– 89.61
n-Hexadecane	226.4	– 67.35	– 67.57	– 0.22	– 94.98	– 94 84
n-Heptadecane	240 4	– 70.99	– 71.19	– 0.20	– 100.23	– 100.07
n-Octadecane	254.5	– 74 64	– 74.84	– 0.20	– 105 48	– 105.34
n-Nonadecane	268.5	– 78 28	– 78.47	– 0.19	– 110.74	– 110 56
n-Eicosane	282.5	– 81.93	– 82.10	– 0.17	– 115.99	– 111 79
			Av.	0 29		

LE 2
paraffins at different temperatures

Diff	API Proj. 44	800°K Calc.	Diff.	API Proj. 44	1200°K Calc.	Diff.
2 37	– 20.82	– 19.06	0.76	– 21.79	– 19.39	2 40
– 0 06	– 24 53	– 24.97	– 0.44	– 25 64	– 25.35	0.29
– 0.35	– 30.12	– 30 89	– 0.77	– 31.16	– 31.31	– 0.15
0.02	– 36.42	– 36.85	– 0.43	– 37.46	– 37.32	0.14
– 0.03	– 42.29	– 42.76	– 0.47	– 43.35	– 43.28	0.07
– 0.01	– 48.28	– 48.72	– 0.44	– 49.35	– 49.28	0.07
0.01	– 54.23	– 54.64	– 0.41	– 55.32	– 55.25	0.07
0.03	– 60.18	– 60.56	– 0.38	– 61.29	– 61.21	0.08
0.02	– 66.12	– 66.52	– 0.40	– 67.25	– 67.22	0.03
0.04	– 72.07	– 72.44	– 0.34	– 73.22	– 73.18	0.04
0.06	– 78.02	– 78.35	– 0.33	– 79.19	– 79.14	0.05
0.08	– 83.97	– 84.25	– 0.28	– 85.16	– 85.10	0.06
0 07	– 89.92	– 90.22	– 0.30	– 91.13	– 91.11	0.02
0 10	– 95.86	– 96.16	– 0 30	– 97.06	– 97.07	0.02
0.12	– 101.81	– 102.05	– 0.24	– 103 06	– 103.03	0.03
0.14	– 107.76	– 107.99	– 0.23	– 109.03	– 109.00	0.03
0.16	– 113.71	– 113.79	– 0.08	– 115.00	– 114.96	0.04
0.14	– 119 66	– 119.89	– 0.23	– 120.97	– 120.96	0.01
0.18	– 125.60	– 125.69	– 0 09	– 126.93	– 126.93	0.00
0.20	– 131.55	– 131.69	– 0.14	– 132.90	– 132.89	0.01
Av. 09			Av. 0.33			Av. 0.06

TABLE

Heat of formation ($\Delta H°_f$) of

Monolefins	Mol. wt.	API Proj 44	0 K Calc.	Diff.	API Proj. 44	400°K Calc.
Ethylene	28.1	14.52	12.51	−2.01	11.77	9.06
Propylene	42.1	8.47	8.82	0.35	3.76	3.87
1-Butene	56.1	4.96	5.14	0.18	−1.49	−1.32
1-Pentene	70.2	1.13	1.43	0.30	−6.77	−6.54
1-Hexene	84.2	−2.54	−2.25	0.29	−12.06	−11.73
1-Heptene	98.2	−6.18	−5 93	0.25	−17.31	−16 99
1-Octene	112.2	−9.83	−9.61	0.22	−22.56	−22.10
1-Nonene	126.2	−13.47	−13.29	0.18	−27.82	−27 28
1-Decene	140 3	−17.12	−17 00	0.12	−33.07	−32.51
1-Undecene	154.3	−20.76	−20.68	0.08	−38.32	−37.69
1-Dodecene	168.3	−24 40	−24 37	0 03	−43.57	−42.88
1-Tridecene	182.3	−28.05	−28.05	0.00	−48.82	−48 07
1-Tetradecene	196 4	−31.69	−31 76	−0.07	−54.08	−53.29
1-Pentadecene	210.4	−35.34	−35.44	−0.10	−59.33	−58.47
1-Hexadecne	224.4	−38 98	−39.12	−0.14	−64.58	−63.66
1-Heptadecene	238.4	−42.62	−42.80	−0.18	−69.83	−68 85
1-Octadecene	252.5	−46.27	−46.51	−0.24	−75.08	−74.08
2-Nonadecene	266.6	−49.91	−50.19	−0.28	−80.34	−79 26
1-Eicosane	280 5	−53.56	−53 87	−0 31	−85.59	−84.44

Av. 18

3
moncolefins at different temperatures

Diff.	API Proj. 44	800°K Calc.	Diff.	API Proj. 44	1200°K Calc.	Diff.
− 2.71	9.70	6.67	3.03	8 88	5 62	3.26
0.11	0.76	0.79	− 0.03	− 0.32	− 0 35	− 0.03
0.17	− 5.15	− 5.10	+ 0.05	− 6.26	− 6.32	− 0.06
0.23	− 11.10	− 11.02	0.08	− 12 20	− 12.33	− 0.13
0.33	− 17.08	− 16.90	0.18	− 18.19	− 18.31	− 0.12
0.40	− 23.03	− 22.79	0.24	− 24.16	− 24.28	− 0 12
0.46	− 28.08	− 28.67	− 0.59	− 30.13	− 30.25	− 0.12
0.54	− 34.92	− 34.55	0.37	− 36.09	− 36.22	− 0.13
0.58	− 40 87	− 40.48	0.39	− 42.06	− 42.24	− 0.18
0.63	− 46.82	− 46.36	0.46	− 48.03	− 48.21	− 0.18
0.69	− 52.77	− 52.25	0.52	− 54.00	− 54.18	− 0.18
0.75	− 58.72	− 58.13	0.59	− 59.97	− 60.15	− 0.18
0.79	− 64 66	− 64.06	0.60	− 65.93	− 66.17	− 0.24
0 86	− 70 61	− 69.94	0.67	− 71.90	− 72.14	− 0.24
0.92	− 76.56	− 75.82	0.74	− 77.87	− 78.11	− 0.24
0 98	− 82.51	− 81.71	0.80	− 83.84	− 84.09	− 0.25
1.00	− 88.46	− 87.63	0.83	− 89 81	− 90.10	− 0 29
1 08	− 94 40	93 51	0 89	− 95.77	− 96.07	− 0.30
1 15	− 100.35	− 99 40	0.95	− 100.74	− 102 04	− 0.30
v 0 65			Av. 0 50			Av. 0.18

TABLE

Heat of formation ($\Delta H°_f$) of

Alkylbenzenes	Mol. wt.	API Proj. 44	0°K Calc.	Diff.	API Proj. 44	400°K Calc.
Benzene	78.1	24.00	21.15	− 2 85	18.55	15.47
Methylbenzene	92.1	17.50	17.39	− 0.11	10.33	10.19
Ethyl ,,	106.1	13.92	13.63	− 0 29	5.22	4.90
n-Propyl ,,	120.2	9.81	9.85	0 04	− 0.34	− 0 43
n-Butyl ,,	134.2	5.93	6.09	0.16	− 5.84	− 5.71
n-Pentyl ,,	148.2	2 28	2.33	0.05	− 11.10	− 11.00
n-Hexyl ,,	162.3	− 1.36	− 1.45	− 0.09	− 16.35	− 16.33
n-Heptyl ,,	176.3	− 5.01	− 5.21	− 0.20	− 21.60	− 21.61
n-Octyl ,,	190.3	− 8.65	− 8.97	− 0.32	− 26.86	− 26 90
n-Nonyl ,,	204.3	− 12.30	− 12.72	− 0.42	− 32.11	− 32.19
n-Decyl ,,	218.4	− 15.94	− 16.51	− 0.57	− 37.36	− 37.51
n-Undecyl ,,	232.4	− 19 58	− 20.27	− 0 69	− 42.61	− 42 80
n Dodecyl ,,	246.4	− 23.23	− 24 02	− 0 79	− 47 86	− 48.09
n-Tri ,,	260.4	− 26.87	− 27.78	− 0.91	− 53.12	− 53.38
n-Tetra ,,	274.5	− 30.52	− 31.56	− 1.04	− 58.37	− 58.70
n-Penta ,,	288.5	− 34.15	− 35.32	− 1.17	− 63.62	− 63.99
n-Hex ,,	302.5	− 37.80	− 39.08	− 1.28	− 68.87	− 69.28

Av. 0.51

4
alkyl benzenes at different temperatures

Diff	API Proj. 44	800°K Calc	Diff.	API Proj. 44	1200°K Calc.	Diff.
– 3.08	15.51	12.31	3.20	14.52	11.08	3 44
– 0.14	6.40	6.40	0.00	5.27	5 09	0.18
– 0.32	0.80	0.49	0.31	– 0.28	– 0.89	– 0.61
– 0.09	– 5.42	– 5.46	– 0.04	– 6.80	– 6 92	– 0.12
0.13	– 11.62	– 11.38	0.24	– 12.70	– 12.90	– 0.20
0.10	– 17.57	– 17.29	0.28	– 18 70	– 18.88	– 0.18
0.02	– 23.52	– 23.24	0 28	– 24.70	– 24.91	– 0.21
– 0.01	– 29.47	– 29.15	0.32	– 30 60	– 30.89	– 0.29
– 0.04	– 35.41	– 35.06	0.35	– 36.60	– 36 88	– 0.28
– 0.08	– 41.36	– 40.97	0.39	– 42.60	– 42 86	– 0 26
– 0 15	– 47.31	– 46.93	0 38	– 48 60	– 48 89	– 0.29
– 0.19	– 53.26	– 52.84	0 42	– 54.50	– 54 87	– 0.37
– 0 23	– 59.21	– 58.75	0.46	– 60.50	– 60.85	– 0.35
– 0.16	– 65.15	– 64.66	0 49	– 66.50	– 66.84	– 0.34
– 0.33	– 71.10	– 70.61	0.49	– 72.40	– 72 86	– 0.46
– 0.37	– 77 05	– 76.52	0.53	– 78.40	– 78.85	– 0 45
– 0.41	– 83.00	– 82.43	0.57	– 84.40	– 84.83	– 0 43
0.17			Av. 0 35			Av. 0.31

TABLE

Heat of formation ($\Delta H°_f$) of

Cyclopentanes	Mol. wt.	API Proj. 44	0°K Calc.	Diff	API Proj. 44	400°K Calc.
Cyclopentane	70.1	−10.68	−13.06	−2.38	−20.80	−22.82
Methyl ,,	84.2	−16.62	−16.74	−0.12	−28.07	−28.10
Ethyl ,,	98.2	−20.23	−20.40	−0.17	−33.29	−33.35
n-Propyl ,,	112.2	−23.98	−24.05	−0.07	−38.64	−38.59
n-Butyl ,,	126.2	−27.52	−27.71	−0.19	−43.79	−43.84
n-Pentyl ,,	140.3	−31.16	−31.39	−0.23	−49.04	−49.12
n-Hexyl ,,	154.3	−34.81	−35.04	−0.23	−54.29	−54.37
n-Heptyl ,,	168.3	−38.45	−38.70	−0.25	−59.55	−59.61
n-Octyl ,,	182.3	−42.10	−42.35	−0.25	−64.80	−64.86
n-Nonyl ,,	196.4	−45.74	−46.04	−0.30	−70.05	−70.14
n-Decyl ,,	210.4	−49.38	−49.69	−0.31	−75.30	−75.39
n-Undecyl ,,	224.4	−53.03	−53.35	−0.32	−80.55	−80.64
n-Dodecyl ,,	238.4	−56.67	−57.00	−0.33	−85.81	−85.88
n-Tridecyl ,,	252.5	−60.32	−60.68	−0.36	−91.06	−91.17
n-Tetra ,,	266.5	−63.96	−64.34	−0.38	−96.31	−96.41
n-Penta ,,	280.5	−67.60	−67.99	−0.39	−101.56	−101.66
n-Hexa ,,	294.5	−71.25	−71.65	−0.40	−106.81	−106.90
				Av. 0.27		

5
cyclopentanes at different temperatures

Diff.	API Proj. 44	800°K Calc.	Diff.	API Proj. 44	1200°K Calc.	Diff.
− 2.02	− 26 06	− 27.59	− 1.53	− 26.97	− 28.22	− 1.25
− 0 03	− 33.74	− 33.50	0.24	− 34.52	− 34.19	0 33
− 0.06	− 39.67	− 39.38	0.29	− 40.34	− 40.11	0.23
0.05	− 45.72	− 45.25	0 47	− 46.40	− 46.04	0.36
− 0.05	− 51.56	− 51.13	0.43	− 52.30	− 51.96	0.34
− 0.08	− 57.51	− 57 05	0.46	− 58.30	− 57.93	0.37
− 0.08	− 63.46	− 62.92	0.54	− 64 20	− 63.86	0.34
− 0.06	− 69.40	− 68.80	0 60	− 70.20	− 69.78	0.42
− 0.06	− 75.35	− 74.67	0.68	− 76 20	− 75.71	0.49
− 0.09	− 81.30	− 80.59	0.71	− 82.20	− 81 68	0.52
− 0 09	− 87.25	− 86.46	0 79	− 88 10	− 87.61	0 49
− 0.09	− 93 20	− 92.34	0.86	− 94.10	− 93 53	0.57
− 0.07	− 99.14	− 98.21	0.93	− 100.10	− 99.46	0.64
− 0.11	− 105.09	− 104.13	0.96	− 106.00	− 105.43	0.57
− 0.10	− 111.04	− 110 00	1.04	− 112.00	− 111.35	0.65
− 0.10	− 116 99	− 115.88	1.11	− 118.00	− 117.28	0.72
− 0 09	− 122.94	− 121.75	1.19	− 123 90	− 123 20	0 70
. 0 07			Av. 0.71			Av. 0 48

TABLE

Heat of formation ($-H°_f$) c

Cyclohexanes	Mol. wt.	API Proj. 44	0°K Calc.	Diff.	API Proj. 44	400°K Calc.
Cyclohexane	84.2	– 20.01	– 21.42	– 1.41	– 31.70	– 33.6
Methyl ,,	98.2	– 26.30	– 25.21	1.09	– 39.79	– 38.81
Ethyl ,,	112.2	– 28.94	– 28.89	0 05	– 44.13	– 44.01
n-Propyl ,,	126.2	– 32.62	– 32.57	0.05	– 49 60	– 49.21
n-Butyl ,,	140.3	– 36.09	– 36 28	– 0.19	– 54.60	– 54 45
n-Pentyl ,,	154.3	– 39.73	– 39.96	– 0.23	– 59.80	– 59.65
n-Hexyl ,,	168.3	– 43.38	– 43.64	– 0.26	– 65.10	– 64.85
n-Heptyl ,,	182.3	– 47.02	– 47.32	– 0 30	– 70.40	– 70.05
n-Octyl ,,	196.4	– 50.67	– 51.03	– 0.36	– 75.60	– 75.29
n-Nonyl ,,	210 4	– 54.31	– 54.71	– 0.40	– 80 80	– 80.49
n-Decyl ,,	224.4	– 57.95	– 58.40	– 0.45	– 86.10	– 85.69
n-Undecyl ,,	238.4	– 61.60	– 62 08	– 0.48	– 91.40	– 90.90
n-Dodecyl ,,	252.5	– 65.24	– 65.79	– 0 55	– 96.60	– 96.13
n-Tridecyl ,,	266.5	– 68.89	– 69.47	– 0.58	– 101.80	– 101.33
n-Tetra ,,	280.5	– 72.53	– 73.15	– 0.62	– 107.10	– 106 54
n-Penta ,,	294.5	– 76 17	– 76.83	– 0 66	– 112.40	– 111.74
n-Hexa ,,	308.6	– 79.82	– 80 54	– 0.72	– 117.60	– 116.97

Av. 0.44

6
cyclohexanes at different temperatures

Diff.	API Proj. 44	800°K Calc.	Diff.	API Proj. 44	1200°K Calc.	Diff.
− 1 91	− 37.19	− 37.62	− 0.43	− 36.68	− 37.19	− 0 51
0.98	− 45.10	− 43.51	1.59	− 44 36	− 43.11	1.25
0.12	− 49 98	− 49.40	0.58	− 49.25	− 49 03	0.22
0.39	− 56.00	− 55.29	0.71	− 55.30	− 54.95	0.35
0.15	− 61.80	− 61.22	0.58	− 61.10	− 60.92	0 18
0.15	− 67.80	− 67.11	0.69	− 67.10	− 66.84	0.26
− 0.75	− 73.70	− 72.99	0 71	− 73.00	− 72.76	0.24
0.35	− 79.60	− 78.88	0.72	− 79.00	− 78.67	0.33
0.31	− 85.60	− 84.81	0.79	− 85.00	− 84.64	0.36
0.31	− 91.60	− 90.70	0.90	− 91.00	− 90.56	0.44
0.41	− 97.50	− 96.59	0.91	− 96.90	− 96.48	0.42
0.50	− 103 40	− 102.48	0.92	− 102.90	− 102.40	0.52
0.47	− 109.40	− 108 41	0 99	− 108.80	− 108.37	0.43
0.47	− 115 40	− 114.30	1.10	− 114.80	− 114.29	0 51
0.56	− 121.30	− 120.19	1.11	− 120.80	− 120 21	0.59
0.66	− 127 20	− 126.07	1.13	− 126.70	− 126.13	0.57
0.63	− 113 20	− 132.00	1.20	− 132.70	− 132 09	0.61
0.45			Av. 0.91			Av. 0.45

TABLE

Heat of formation ($\Delta H°_f$) of normal

n-Acetylenes	Mol. wt.	API Proj. 44	0°K Calc.	Diff.	API Proj. 44	400°K Calc.
Ethyne	26.0	54.33	49 67	− 4 67	54.13	48.83
Propyne	40.1	46.02	46.02	0.00	43.77	43.57
1-Butyne	54.1	42.74	42.39	− 0.35	38 57	38.34
1-Pentyne	68.1	38.90	38.77	− 0.13	33.28	33.11
1-Hexyne	82.1	35.26	35.14	− 0 12	28.03	27.87
1-Heptyne	96.2	31.61	31.48	− 0.13	22.78	22.61
1-Octyne	110.2	27.97	27.86	− 0.11	17.52	17.37
1-Nonyne	124.2	24.32	24.23	− 0.09	12.27	12.14
1-Decyne	138 2	20.68	20.60	− 0 08	7.02	6.91
1-Undecyne	152 3	17.04	16.95	− 0.09	1.77	1.64
1-Dodecyne	166.3	13.39	13.32	− 0.07	− 3.48	− 3.59
1-Tridecyne	180.3	9.75	9.69	− 0 06	− 8 74	− 8 82
1-Tetra „	194.3	6.10	6 07	− 0.03	− 13.99	− 14.05
1-Penta „	208 4	2.46	2.41	− 0 05	− 19 24	− 19.32
1-Hexa „	222.4	− 1.18	− 1.21	− 0.03	− 24.49	− 24.55
1-Hepta „	236.4	− 4.83	− 4.84	− 0.01	− 29 74	− 29.78
1-Octa „	250.4	− 8.47	− 8.47	0.00	− 35.00	− 35.01
1-Nona „	264.5	− 12.12	− 12.12	0.00	− 40.25	− 40.28
1-[illegible]	278.5	− 15.76	− 15.75	0.01	− 45.50	− 45.51

Av. 0.07

7
acetylenes at different temperatures

Diff.	API Proj. 44	800°K Calc.	Diff.	API Proj. 44	1200°K Calc.	Diff.
− 5.30	53.63	48.23	− 5.40	53.00	47.42	5 58
− 0.20	42 07	42.27	0.20	41.49	41.38	0 19
− 0.23	36.04	36.35	0.31	35.05	35.37	0.32
− 0.17	30.09	30.43	0.33	29.10	29.37	0.27
− 0.16	24.14	24.51	0.37	23.13	23.37	0.24
− 0.17	18.19	18.55	0.34	17.16	17.32	0.16
− 0.15	12.25	12.64	0.39	11.20	11.31	− 0.11
− 0.13	6.30	6.72	0.42	5.23	5.31	0.08
− 0 11	0.35	0 80	0.45	− 0 74	− 0.69	0.05
− 0.13	− 5 60	− 5.16	0.44	− 6.71	− 6.74	− 0.03
− 0 11	− 11.55	− 11.07	0.48	− 12.67	− 12.74	− 0.07
− 0.08	− 17 49	− 16.99	0.50	− 18.64	− 18.74	− 0.10
− 0.06	− 23.44	− 22.91	0 53	− 24.61	− 24.75	− 0.14
− 0.08	− 29.39	− 28 87	0.52	− 30 58	− 30 80	− 0.22
− 0.06	− 35.34	− 34.79	0.55	− 36.55	− 36.80	− 0.25
− 0.04	− 41.29	− 40 70	0 59	− 42 51	− 42.80	− 0.29
− 0.01	− 47.23	− 46 62	0 61	− 48.48	− 48 81	− 0.33
− 0.03	− 53.18	− 52.58	0.60	− 54.45	− 54 85	− 0.40
− 0.01	− 59.13	− 58 50	0.63	− 60.42	− 60 86	− 0.44
Av. 0.11			Av. 0.46			Av. 0.20

REFERENCES

1. Reid, R. C. and T. K. Sherwood .. "Properties of gases and liquids", 2nd Edition. McGraw Hill, 1966.
2. Ibrahim, S. H. and N. R. Kuloor . *Chem Engg.*, 1966, 73(25), 147.
3. Pachaiyappan, V., Ibrahim, S. H. and Kuloor, N. R. *Ibid.*, 1967, 74(4), 140.
4. ——— ——— .. .. *Ibid.*, 1967, 74(11), 193.
5. ——— ——— .. .. *Ibic.*, 1967, 74(21), 241.
6. ——— ——— .. .. *Ibid.*, 1967, 74(22), 172.
7. Das, T. R., Ibrahim, S. H. and N. R. Kuloor. Communicated to Chem. Engg.
8. ——— ——— .. .. Communicated to Chem Engg.
9. American Petroleum Institute Project 44 Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds. Carnegie Press, Pittsburgh Pa (1953) and Supplements.