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### Publication Date

1986-08-01



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P.A. Rodgers, A.L. Creagh, and J.M. Prausnitz

August 1986

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*Correlation of Liquid Heat Capacities for  
Fossil Fuels Using Characterization Data*

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This work was supported by the Director, Office of Energy Research, Office of Basic Energy Science, Chemical Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

## ABSTRACT

Heat capacities for liquid fossil-fuel fractions are correlated as a function of characterization data. The correlation uses molecular weight from freezing-point-depression or gel-permeation-chromatography measurements, molar hydrogen-to-carbon ratio from elemental analysis, hydrogen distribution from proton-nuclear-magnetic-resonance data, and if available, number of methyl, hydroxyl, primary amine, and secondary amine groups per molecule from IR spectroscopy. The correlation is established for temperatures below 500 K using characterization data for 118 pure hydrocarbons; the average deviation from experiment is 2.3 percent. When the correlation is used to predict the heat capacities of nine petroleum fractions, the average deviation is 2.6 percent. Average deviations for fourteen coal-derived liquids are about 6.5 percent, but for those liquids containing more than about 3 weight-percent oxygen, the average deviation is somewhat lower. For high-oxygen-containing fractions, the correlation presented here is significantly better than that of Mraw et al.

## Introduction

Heat capacities for fossil fuels are required for heat-balance calculations such as those for design of heat exchangers or distillation columns. To reduce energy costs for processing of fuels, it is desirable to predict accurate heat capacities for petroleum fractions and coal-derived liquids.

As discussed by Tsonopoulos et al (1), there are basically four types of correlations for predicting liquid heat capacities: theoretical, corresponding-states, group-contribution, and empirical. Reid et al (2) point out that reliable theoretical procedures for predicting liquid heat capacities have not yet been developed for engineering applications. Although corresponding-states and group-contribution methods (3-5) have proved to be satisfactory for defined compounds, they cannot easily be applied to petroleum and coal-derived liquids, because of a lack of information on molecular structure and critical properties. To obtain the group concentrations necessary for the group-contribution methods, much experimental effort is required for separation and subsequent analysis of the fractions, as pointed out by Le and Allen (5). Further, most corresponding-states methods also require the ideal-gas heat capacity to predict the liquid heat capacity of a compound or mixture. Although known accurately for most defined compounds, the ideal-gas heat capacity of fractions must be predicted from other correlations. Consequently, additional error is introduced in the final predicted liquid heat capacity.

Conventional methods for correlating liquid heat capacities for fossil fuels are based on the Watson K factor and specific gravity (6); these methods are modified forms of a correlating equation presented over fifty years ago by Watson and Nelson (7).

This work presents a correlation for liquid heat capacity that can be applied to petroleum fractions and coal-derived liquids for temperatures below 500 K. Data for 118 pure hydrocarbons, including normal, branched and cyclic alkanes, and aromatic compounds, were used to establish a correlation based on characterization data. For pure substances, these data are available upon inspection; for fractions they are obtained by well-defined chemical-analytical methods, as discussed elsewhere (8,9). Characterization data include molecular weight, molar hydrogen-to-carbon ratio, and hydrogen distribution. For fossil-fuel fractions, molecular weight is obtained from freezing-point depression or gel-permeation-chromatography data; the H/C ratio is obtained from elemental analysis, and the hydrogen distribution is obtained from proton-nuclear-magnetic-resonance spectroscopy data.

To predict liquid heat capacities for coal-derived liquids, it is necessary to take into account heteroatomic groups. Using data for 23 oxygen-, nitrogen-, and sulfur-containing compounds, the correlation established for hydrocarbons was extended to apply also for heteroatomic hydrocarbon derivatives.

#### Liquid Heat-Capacity Correlations: Background

Reid et al (2) give three definitions for liquid heat capacities. The liquid heat capacity of interest here is  $C_p$ , the enthalpy change with temperature at constant pressure.

For hydrocarbon mixtures, Reid et al (2) recommend the correlations of Luria and Benson (10) and of Hadden (11,12).

Luria and Benson (10) developed a group-contribution method for determining liquid heat capacities for hydrocarbons below the normal boiling point. Data for 117 hydrocarbons were used to obtain

polynomial expressions (cubic in temperature) for 20 hydrocarbon groups and 12 molecular-structural features. The liquid heat capacity for a compound is found by adding the polynomial expressions for the groups that constitute the compound; 1209 independent data points were reproduced using this method. The average absolute deviation between calculated and observed values was 2.7 J/gmol-K.

Hadden (11) tested a modified Watson-Nelson correlation for normal alkanes and found poor agreement between experimental and calculated heat capacities. Hadden (12) also presented empirical relations for the liquid heat capacities of pure liquid hydrocarbons for temperatures to the normal boiling point. Dimensionless equations were developed for members of a homologous series: n-alkanes, isoalkanes, 1-alkenes, alkylcyclo-hexanes, alkylcyclopentanes and alkylbenzenes. A separate correlation was given for light alkanes from methane through butane. Deviations of experimental from calculated liquid heat capacities were less than 1 percent.

For the calculation of liquid heat capacities of petroleum fractions, the correlation of Watson and Nelson (7) is often used:

$$C_p = (0.35 + 0.055K_w) \left[ 0.6811 - 0.308s + (0.815 - 0.306s) \frac{t}{1000} \right] \quad (1)$$

where  $C_p$  is the liquid heat capacity in BTU/lb<sub>m</sub>°F;  $t$  is the temperature in °F;  $s$  is the specific gravity at 60/60°F and  $K_w$  is the Watson K factor calculated from:

$$K_w = \sqrt[3]{T_b} / s \quad (2)$$

where  $T_b$  is the normal boiling point in °R.

The API Technical Data Book (13) presents a similar equation



using  $K_w$  and specific gravity. The heat capacity is a quadratic function of temperature.

Mraw et al (6) modified the Watson-Nelson equation to cover coal liquids:

$$C_p = (0.06759 + 0.05638K_w) \left[ 0.6450 - 0.05959s + (1.2892 - 0.5264s) \frac{t}{1000} \right] \quad (3)$$

One disadvantage of using Equations (1) and (3) is that the boiling point of the fraction is required to obtain the Watson K factor. For high-boiling fractions, it is necessary to perform a vacuum distillation to obtain a boiling curve (eg. ASTM Method D 1160) and to apply corrections to obtain the "true" distillation curve. The boiling point is arbitrarily taken to be the 50-percent-distilled temperature on this curve.

Recently, Le and Allen (5) presented a group-contribution method for the estimation of heat capacities of coal-derived liquids. Group concentrations are determined using data from chromatographic separations, elemental analysis,  $^1\text{H-NMR}$ ,  $^{13}\text{C-NMR}$ , and mass spectrometry. Heat-capacity estimates of coal-liquid fractions showed an average absolute deviation of less than 3 percent from experiment, but at high temperatures (above 400 K), the accuracy of this method decreases, reaching deviations of roughly 20 percent.

#### Heat Capacity Correlation Using Characterization Data

This work presents a correlation for liquid heat capacities of petroleum fractions and coal-derived liquids. Using a least-squares program, 2969 liquid heat-capacity data for 118 pure hydrocarbons (carbon numbers greater than or equal to five) were linearly regressed to obtain a function of temperature and the characterization data

indicated above. Data used in the correlation are summarized in Appendix A. The H/C ratio is obtained from elemental analysis, while the hydrogen distribution is obtained from proton-nuclear-magnetic-resonance data; it is normalized to include only alpha (1.7-4.0 ppm shift), beta (0.9-1.7 ppm), gamma (0.5-0.9 ppm), and aromatic-type (6.0-9.0 ppm) hydrogen atoms. The 4.0-6.0 ppm shift range, which covers olefinic and phenolic hydrogens, is not taken into account here. The normal boiling point is not required.

The correlation gives liquid heat capacity as a function of temperature :

$$C_p = A + B T + C T^2 \quad (4)$$

where  $C_p$  is the liquid heat capacity in J/kg-K;  $T$  is the temperature in K;  $A$ ,  $B$ , and  $C$  are coefficients which depend on characterization data.

Equation (4) is quadratic in temperature. As discussed in Appendix B, several other forms were investigated; these included functions of  $1/T$  and functions of reduced temperatures,  $T/T^*$  and  $T/T_b$ , where  $T^*$  is a reducing temperature used in the perturbed-hard-chain equation of state (14,15);  $T_b$  is the normal boiling-point in K. Performance of the various forms, in terms of average deviation from experiment, were about equal.  $T$  was chosen as the temperature variable because it extrapolates to higher temperatures better than the other forms.

We distinguish between two cases: In the first, we use characterization data from elemental analysis, molecular-weight determination, and proton-nuclear-magnetic-resonance spectra ( $^1\text{H-NMR}$ ); in that event, the coefficients are given by:

$$A = A_0 MW + A_1 H/C + A_2 H_\alpha + A_3 H_\beta + A_4 H_\gamma \quad (4a)$$

$$B = B_0 + B_1 H/C + B_2 H_\alpha + B_3 H_\beta + B_4 H_\gamma \quad (4b)$$

$$C = C_0 + C_1 MW + C_2 H_\alpha + C_3 H_\gamma \quad (4c)$$

where MW is molecular weight in g/mol; H/C is the molar hydrogen-to-carbon ratio from elemental analysis;  $H_\alpha$  is the fraction of hydrogen atoms attached to a carbon that is alpha to an aromatic ring;  $H_\beta$  is the fraction of hydrogen atoms attached to a carbon that is beta or further, but non-terminal, to an aromatic ring;  $H_\gamma$  is the fraction of hydrogen atoms attached to terminal carbons.

In the second case, hydrogen-distribution ( $^1\text{H-NMR}$ ) data are not used. This case is of practical importance because unfortunately, at present,  $^1\text{H-NMR}$  data are only rarely available for fractions. In the absence of hydrogen-distribution data, the coefficients are given by:

$$A = A_0 + A_1 MW + A_2 H/C \quad (4d)$$

$$B = B_0 MW + B_1 H/C \quad (4e)$$

$$C = C_0 + C_1 MW + C_2 H/C \quad (4f)$$

Table 1 gives the coefficients in Equations (4a) through (4f) as well as the correlation coefficients and the average deviation from experiment. For pure hydrocarbons, the average deviation for Equation (4) with Equations (4a-4c) is 2.3 percent, with a maximum deviation of 12.0 percent. Equation (4) with Equations (4d-4f) gives an average deviation of 4.2 percent, with a maximum deviation of 18.4 percent.

#### Heteroatomic Correction

To account for the presence of heteroatomic groups, corrections are added to Equation (4):

$$C_p = C_{pHC} + \Delta C_{pO} + \Delta C_{pN} + \Delta C_{pS} \quad (5)$$

where  $C_{pHC}$ , the hydrocarbon heat capacity, is calculated from Equation (4); the corrections are given by:

$$\Delta C_{pO} = [a_0 + a_1 MW + a_2 H/C + a_3 z_{OH} + a_4 T] [O/C] \quad (5a)$$

$$\Delta C_{pN} = [b_0 + b_1 MW + b_2 H/C + b_3 (z_{NH} + z_{NH_2}) + b_4 T] [N/C] \quad (5b)$$

$$\Delta C_{pS} = [c_0 + c_1 MW + c_2 H/C + c_3 z_{CH_3} + c_4 T] [S/C] \quad (5c)$$

where H/C, O/C, N/C, and S/C are, respectively, the molar ratios of hydrogen, oxygen, nitrogen, and sulfur to carbon;  $z_{OH}$ ,  $z_{NH_2}$ ,  $z_{NH}$ , and  $z_{CH_3}$  are, respectively, the number of hydroxyl, primary amine, secondary amine, and methyl groups per molecule; and T is the temperature in K. Functional-group concentrations are determined using infrared spectroscopy as described elsewhere (8).

If elemental analysis is available but functional-group concentrations are not, the corrections are given by:

$$\Delta C_{pO} = [a_0 + a_1 MW + a_2 H/C + a_3 T] [O/C] \quad (5d)$$

$$\Delta C_{pN} = [b_0 + b_1 MW + b_2 H/C + b_3 T] [N/C] \quad (5e)$$

$$\Delta C_{pS} = [c_0 + c_1 MW + c_2 H/C + c_3 T] [S/C] \quad (5f)$$

Data for 23 pure compounds containing heteroatomic groups were used to determine the coefficients in Equations (5a) through (5f). Table 2 gives the coefficients for the heteroatomic corrections when used with Equations (4) and (4a-4c). Table 3 gives the coefficients for the heteroatomic corrections when used with Equations (4) and (4d-4f).

Table 4 compares six cases for predicting liquid heat capacities

depending on the information available. The first case predicts liquid heat capacities using hydrogen-distribution data [Equation (4) with (4a-4c)], but omits heteroatomic corrections. The average deviation between experimental and predicted liquid heat capacities for the 23 pure heteroatomic compounds is 28.2 percent, with a maximum of 114 percent.

The second case incorporates the heteroatomic correction factors with functional-group concentrations [Equations (4) with (4a-4c), (5) with (5a-5c)]. This reduces the average deviation between predicted and observed values to 2.8 percent, with a maximum of 11.4 percent.

Case three uses heteroatomic corrections without functional-group concentrations [Equations (4) with (4a-4c), (5) with (5d-5f)]. The average deviation is now 5.2 percent, with a maximum of 18.9 percent.

The fourth case predicts liquid heat capacities without hydrogen-distribution data [Equation (4) with (4d-4f)] and without heteroatomic corrections. The average deviation between experimental and predicted liquid heat capacities is 19.4 percent, with a maximum of 48.9 percent.

The fifth case incorporates heteroatomic corrections with functional-group concentrations [Equations (4) with (4d-4f), (5) with (5a-5c)]. The average deviation is now 4.9 percent, with a maximum of 25.2 percent.

Case six uses heteroatomic corrections without functional-group concentrations [Equations (4) with (4d-4f), (5) with (5d-5f)]. The average deviation increases slightly to 5.2 percent, with a maximum of 22.6 percent.

For compounds containing heteroatomic groups, Equation (4) with (4d-4f) but without heteroatomic corrections gives liquid heat

capacities better than those from Equation (4) with (4a-4c), probably because the hydrogen distribution used in Equations (4a-4c) is normalized to include only the types of hydrogen atoms mentioned immediately after Equation (4c). Heteroatomic groups often include hydrogen atoms which are not accounted for in the normalization. However, the inclusion of heteroatomic corrections, with or without hydrogen-distribution data, significantly improves prediction of liquid heat capacities for compounds containing heteroatomic groups.

#### Heat Capacities of Fossil-Fuel Fractions

Since it is difficult to find heat-capacity data for petroleum fractions or coal-derived liquids that have been well characterized (i.e.  $^1\text{H-NMR}$  data and heteroatomic functional-group concentrations), it is not possible to test the correlation using coefficients calculated from Equations (4a-4c) or (5a-5c). However, Equation (4) with Equations (4d-4f) was tested using petroleum-fraction enthalpy data of Lenoir and Hipkin (16,17). Equations (5) and (5d-5f) were applied to enthalpy and heat-capacity data for coal-derived liquids reported by Yesavage et al (18), Gray et al (19), and by Mraw et al (6). Table 5 gives limited characterization data for these fractions.

From the data available, it is sometimes difficult to obtain accurate liquid heat capacities. Lenoir and Hipkin (16,17) and Yesavage et al (18) report enthalpies as a function of temperature. To obtain heat capacities, the liquid enthalpy data were first regressed (cubic in temperature) and then differentiated, giving a smooth estimate for heat capacity. However, Gray et al (19) report liquid-heat-capacity data directly. Mraw et al (6) report smoothed heat capacities.

Table 6 compares experimental and correlated liquid heat capacities. All of the methods appear to be equally good for petroleum fractions; the average deviation for Equations (4,4d-4f) was 2.6 percent compared to 1.6 percent and 5.2 percent for Equations (1) and (3) respectively. While the method of Mraw et al (Equation 3) is significantly better for predicting liquid heat capacities for coal-derived liquids, notable exceptions to this occur for fractions with high oxygen content (ie. greater than 3 weight-percent); for these fractions (SRC-II cuts 6 and 8), Equations (4,4d-4f) with heteroatomic corrections [Equations (5,5d-5f)] give the best results.

Figure 1 compares calculated and observed liquid heat capacities of a typical petroleum fraction as a function of temperature. Figure 1 also shows that for a high-oxygen, coal-derived liquid, the correlation presented here provides a better estimate of heat capacity than that of Mraw et al (6).

Mraw et al (6) did not include phenolic compounds in their correlation; for such compounds, they found large deviations when using Equation (3). When Equations (5,5a-5c) with heteroatomic corrections [Equations (5,5a-5c)] were used to calculate heat capacities for phenol and other pure heteroatomic compounds, agreement was much better than that obtained by Mraw et al (6); the results are shown in Table 7. For oxygen-containing compounds, the average deviation using Equations (4,4a-4c) and (5,5a-5c) is 3.0 percent; for nitrogen-containing compounds it is 5.0 percent, while sulfur-containing compounds give an average deviation of 1.2 percent. By contrast, using Equation (3), average deviations are 23.2, 14.7, and 6.6 percent for oxygen, nitrogen, and sulfur-containing compounds, respectively.

### Conclusions

A correlation has been presented to estimate liquid heat capacities for fossil-fuel fractions. This correlation uses characterization parameters obtained from standard chemical-analytical methods. The correlation gives heat capacities for nine petroleum fractions and fourteen coal-derived liquids with an average deviation of 2.6 to 6.5 percent.

The effect of heteroatoms is accounted for by adding corrections to the heat-capacity correlation for pure hydrocarbons. These corrections significantly improve prediction, especially for oxygen-containing compounds.

### Acknowledgments

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. Additional support was provided by the American Petroleum Institute and by the National Science Foundation.

The authors thank Dr. Bruce Gammon of the National Institute for Petroleum and Energy Research (Bartlesville, Oklahoma) for advice and for providing much of the liquid heat-capacity data.



<u>Table</u>	<u>Title</u>
1	Liquid Heat Capacity-Correlation
2	Heteroatomic Corrections to Liquid Heat-Capacity Correlation: Equation (4) with (4a-4c)
3	Heteroatomic Corrections to Liquid Heat-Capacity Correlation: Equation (4) with (4d-4f)
4	Comparison of Liquid Heat-Capacity Correlations with and without Heteroatomic Corrections
5	Characterization Data for Fossil-Fuel Fractions
6	Comparison of Liquid Heat-Capacity Predictions for Petroleum Fractions and for Coal-Derived Liquids
7	Comparison of Liquid Heat-Capacity Predictions for Pure Heteroatomic Compounds
A-1	Liquid Heat-Capacity Data Sources for Pure Hydrocarbons
A-2	Liquid Heat-Capacity Data Sources for Pure Heteroatomic Compounds
B-1	Liquid Heat-Capacity Regression Summary

<u>Figure</u>	<u>Caption</u>
1	Liquid Heat Capacities for a Typical Petroleum Fraction and for a High-Oxygen, Coal-Derived Liquid

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TABLE 1. LIQUID HEAT-CAPACITY CORRELATION

Equation	Coefficient	Coefficient Subscript				
		0	1	2	3	4
(4a)	A	3.12	$2.09 \times 10^3$	$-2.74 \times 10^3$	$-2.81 \times 10^3$	$-3.94 \times 10^3$
(4b)	B	-1.27	-3.38	9.80	6.11	$1.10 \times 10$
(4c)	C	$1.12 \times 10^{-2}$	$-2.05 \times 10^{-5}$	$-8.33 \times 10^{-3}$	$-4.40 \times 10^{-3}$	
(4d)	A	$5.69 \times 10^2$	-3.11	$4.98 \times 10^2$		
(4e)	B	$2.47 \times 10^{-2}$	$-3.93 \times 10^{-1}$			
(4f)	C	$5.57 \times 10^{-3}$	$-4.35 \times 10^{-5}$	$9.21 \times 10^{-4}$		

<u>Equations</u>	<u>Avg. % Deviation</u>	<u>R<sup>2</sup> (a)</u>
(4), (4a-4c)	2.3	0.9993
(4), (4d-4f)	4.2	0.8273

(a) Proportion of the total variance accounted for by the correlation, also known as the correlation coefficient.

TABLE 2. HETEROATOMIC CORRECTIONS TO LIQUID HEAT-  
CAPACITY CORRELATION: EQUATION (4) WITH (4a-4c)

Equation	Coefficient	Coefficient Subscript				
		0	1	2	3	4
(5a)	a	$1.04 \times 10^4$	$5.19 \times 10^2$	$-4.98 \times 10^4$	$-1.18 \times 10^4$	$1.30 \times 10$
(5b)	b	$-3.27 \times 10^3$	$1.47 \times 10$	$1.02 \times 10^3$	$8.33 \times 10^2$	1.24
(5c)	c	$2.97 \times 10^3$	-6.78	$-4.40 \times 10^2$	$-1.32 \times 10^3$	-6.28
(5d)	a	$-2.50 \times 10^4$	$-4.61 \times 10$	$2.37 \times 10^4$	$1.57 \times 10$	
(5e)	b	$-4.77 \times 10^3$	$2.73 \times 10$	$1.06 \times 10^3$	3.17	
(5f)	c	$1.93 \times 10^3$	8.37	$-1.75 \times 10^3$	-5.65	

TABLE 3. HETEROATOMIC CORRECTIONS TO LIQUID HEAT-  
CAPACITY CORRELATION: EQUATION (4) WITH (4d-4f)

Equation	Coefficient	Coefficient Subscript				
		0	1	2	3	4
(5a)	a	$2.08 \times 10^4$	$6.32 \times 10^2$	$-6.36 \times 10^4$	$-1.42 \times 10^4$	2.07
(5b)	b	$4.86 \times 10^3$	$-2.30 \times 10$	$-4.04 \times 10^2$	$1.94 \times 10^3$	-6.49
(5c)	c	$2.97 \times 10^3$	3.30	$-9.25 \times 10^2$	$-5.44 \times 10^2$	-9.17
(5d)	a	$-2.18 \times 10^4$	$-4.86 \times 10$	$2.48 \times 10^4$	5.36	
(5e)	b	$1.34 \times 10^3$	6.53	$-2.91 \times 10^2$	-1.99	
(5f)	c	$2.55 \times 10^3$	9.59	$-1.47 \times 10^3$	-8.92	

TABLE 4. COMPARISON OF LIQUID HEAT-CAPACITY CORRELATIONS  
WITH AND WITHOUT HETEROATOMIC CORRECTIONS

Case	Equations	Percent Deviation (a)	
		Average	Maximum
1	(4), (4a-4c)	28.2	114.
2	with (5), (5a-5c)	2.8	11.4
3	with (5), (5d-5f)	5.2	18.9
4	(4), (4d-4f)	19.4	48.9
5	with (5), (5a-5c)	4.9	25.2
6	with (5), (5d-5f)	5.2	22.6

(a) for 23 heteroatomic compounds

TABLE 5. CHARACTERIZATION DATA FOR FOSSIL-FUEL FRACTIONS

<u>Data Source</u>	<u>Fraction</u>	<u>Avg. MW</u>	<u>H/C</u>	<u>s (a)</u>	<u>K<sub>w</sub></u>
Lenoir & Hipkin (16)	Alaska Naphtha	131	1.892	0.7775	11.63
	Jet Naphtha	144	1.932	0.8044	11.48
	Aromatic Naphtha	126	1.296	0.8524	10.50
	Low-Boiling Naphtha	120	2.086	0.7393	12.10
	High-Boiling Naphtha	142	2.037	0.7620	12.10
	Kerosine	162	1.972	0.8086	11.80
	Fuel Oil (No.2)	228	1.796	0.8602	11.68
	Gas Oil	214	1.846	0.8483	11.80
Lenoir & Hipkin (17)	California Light Naphtha	102	2.042	0.7365	11.94
Yesavage et al (18)	SRC-I Naphtha	132	1.833	0.7809	11.23
Gray et al (19)	SRC-II Narrow-Boiling Coal Liquids				
	cut 2	95	1.847	0.7701	11.37
	cut 4	114	1.699	0.8125	11.12
	cut 6	127	1.353	0.9538	9.91
	cut 8	158	1.280	0.9761	10.05
	cut 10	166	1.209	0.9972	10.13
	cut 12	246	1.027	1.0793	9.76
	cut 14	189	1.132	1.0184	9.92
	cut 15	214	1.030	1.0773	9.74
	cut 17	251	0.977	1.1195	9.70
cut 19	320	0.843	1.1950	9.43	
Mraw et al (6)	Exxon Donor Solvent WA-5	176	1.197	0.9695	10.14
	Exxon Donor Solvent WA-6	186	1.235	0.9865	10.02
	Exxon Donor Solvent WV-1	191	1.179	0.9975	9.96

(a) specific gravity at 60/60°F

TABLE 6. COMPARISON OF LIQUID HEAT-CAPACITY PREDICTIONS  
FOR PETROLEUM FRACTIONS AND FOR COAL-DERIVED LIQUIDS

Data Source	Fraction	Percent Deviation			
		(4) <sup>1</sup>	(4,5) <sup>2</sup>	Watson <sup>3</sup>	Mraw <sup>4</sup>
Lenoir & Hipkin (16)	Alaska Naphtha	2.3	—	2.1	5.2
	Jet Naphtha	0.9	—	0.6	3.9
	Aromatic Naphtha	2.6	—	2.7	6.0
	Low-Boiling Naphtha	2.0	—	3.3	5.5
	High-Boiling Naphtha	3.7	—	1.5	4.7
	Kerosine	2.2	—	0.7	5.3
	Fuel Oil (No.2)	3.4	—	1.3	7.9
	Gas Oil	3.0	—	0.3	5.8
Lenoir & Hipkin (17)	California Light Naphtha	2.9	—	2.3	3.0
	Petroleum Fractions Avg.	2.6	—	1.6	5.2
Yesavage et al (18)	SRC-I Naphtha	4.9	9.6	2.3	0.6
Gray et al (19)	SRC-II Narrow-Boiling Coal Liquids				
	cut 2	1.2	3.3	3.4	3.9
	cut 4	6.4	5.7	4.4	2.2
	cut 6	11.3	7.1	17.3	12.3
	cut 8	8.9	2.9	13.8	7.3
	cut 10	5.3	3.3	9.8	1.7
	cut 12	4.8	8.8	12.0	1.1
	cut 14	6.0	6.2	11.1	2.5
	cut 15	6.6	9.2	14.1	3.3
	cut 17	6.5	11.6	15.5	2.7
cut 19	7.6	17.8	18.5	2.7	
Mraw et al (6)	Exxon Donor Solvent WA-5	2.1	1.9	4.6	2.7
	Exxon Donor Solvent WA-6	1.9	2.0	5.6	2.2
	Exxon Donor Solvent WV-1	1.4	1.1	6.4	1.7
	Coal-Derived Liquids Avg.	5.3	6.5	9.9	3.3

— Not calculated because the heteroatom content is too low

- 1 Equation (4) with (4d-4f)
- 2 Equation (4) with (4d-4f) and Equation (5) with (5d-5f)
- 3 Equation (1)
- 4 Equation (3)



TABLE 7. COMPARISON OF LIQUID HEAT-CAPACITY PREDICTIONS  
FOR PURE HETEROATOMIC COMPOUNDS

Heteroatomic Compound	Average Percent Deviation		Mraw
	Equations (4,4a-4c)		
	no correction	with correction (a)	
o-Cresol	15.9	3.5	24.2
m-Cresol	15.7	2.6	22.9
p-Cresol	15.8	1.9	22.4
Phenol	15.1	0.2	27.7
Furan	13.4	2.7	13.7
Catechol	102.7	5.8	29.9
Hydroquinone	112.7	4.5	21.8
Average Dev. for Oxygen Compounds	41.6	3.0	23.2
Pyrrolidine	5.1	9.5	25.2
Pyrrole	9.1	11.4	15.9
2-Methyl Pyridine	3.9	0.2	5.8
Pyridine	8.4	2.4	7.4
Aniline	4.3	1.4	19.3
Average Dev. for Nitrogen Compounds	6.2	5.0	14.7
Cyclohexanethiol	4.8	0.9	4.6
3-Methyl Thiophene	14.3	2.3	5.3
2-Pentanethiol	37.3	0.6	9.3
3-Pentanethiol	38.5	0.7	6.3
1-Hexanethiol	16.6	1.4	8.0
2-Hexanethiol	31.8	0.4	8.8
1-Heptanethiol	15.2	1.1	7.2
1-Decanethiol	10.1	2.0	3.1
Average Dev. for Sulfur Compounds	21.1	1.2	6.6

(a) Heteroatomic corrections using Equation (5)  
with Equations (5a-5c)

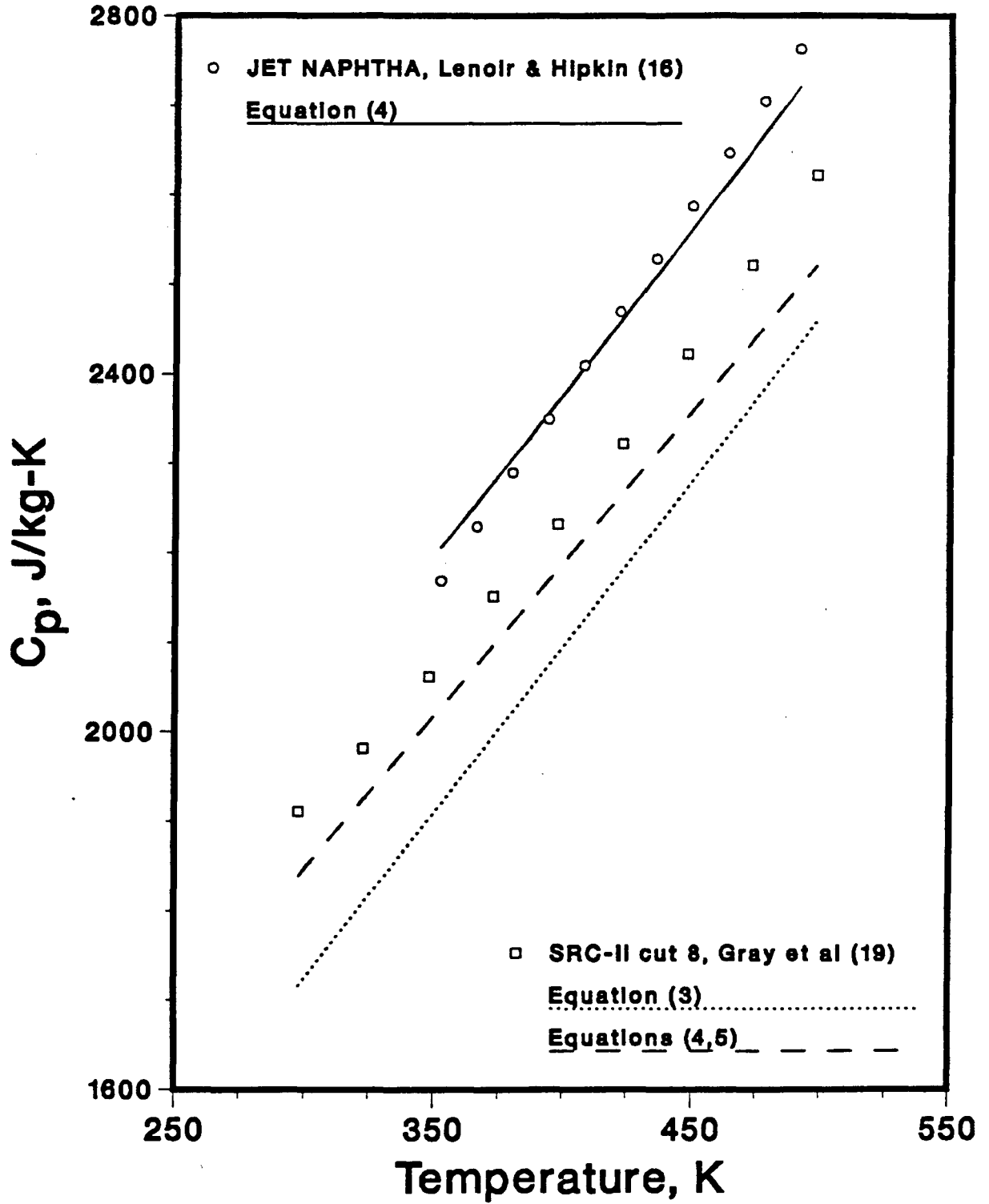


FIGURE 1. Liquid Heat Capacities For A Typical Petroleum Fraction And For A High-Oxygen, Coal-Derived Liquid

## APPENDIX A

## LIQUID HEAT-CAPACITY DATA SOURCES

For correlating liquid heat capacities, 2969 data for 118 pure hydrocarbons were used. Table A-1 gives the number of data points and the data source for each compound.

For correlating heteroatomic corrections to the hydrocarbon liquid heat-capacity estimates, 426 data for 23 pure heteroatomic compounds were used. Table A-2 gives the number of data points and the data source for each compound.

TABLE A-1. LIQUID HEAT-CAPACITY DATA SOURCES FOR PURE HYDROCARBONS

COMPOUND	NUMBER	
	DATA PTS	DATA SOURCE
n-pentane	17	D. Peng and L.I. Stiel AIChE Symposium Series No. 140, 1974, vol 70, p 63 (pressure=400psia)
n-pentane	25	J.F. Messerly, G.B. Guthrie, S.S. Todd and H.L. Finke J Chem and Eng Data, 12, 3, 338 (1967)
n-hexane	33	B. Kalinowska, J. Jedlinska, W. Woycicki and J. Stecki J Chem Thermo, 12, 891 (1980)
n-hexane	13	T.J. Connelly, B.H. Sage and W.N. Lacey Ind and Eng Chem, 43, 4, 946 (1951) (smoothed data)
n-hexane	24	D.R. Douslin and H.M. Huffman J Amer Chem Soc, 68, 1704 (1946)
n-hexane	5	H.M. Huffman, G.S. Parks and M. Barmore J Amer Chem Soc, 53, 3876 (1931)
n-hexane	8	G.S. Parks, H.M. Huffman and S.B. Thomas J Amer Chem Soc, 52, 1032 (1930)
n-hexane	15	Table 23-2-(1.201)-vc API 44, Oct. 31, 1975
n-heptane	96	B. Kalinowska, J. Jedlinska, W. Woycicki and J. Stecki J Chem Thermo, 12, 891 (1980)

n-heptane	8	J.L. San Jose, G. Mellinger and R.C. Reid J Chem Eng Data, 21, 4, 414 (1976)
n-heptane	15	J.C. van Miltenburg J Chem Thermo, 4, 773 (1972) (smoothed data)
n-heptane	22	H.M. Huffman, M.E. Gross, D.W. Scott and J.P. McCullough J Phys Chem, 65, 495 (1961) (smoothed data)
n-heptane	36	D.C. Ginnings and G.C. Furukawa J Amer Chem Soc, 75, 522 (1953) (smoothed data)
n-heptane	14	G.S. Parks, H.M. Huffman and S.B. Thomas J Amer Chem Soc, 52, 1032 (1930)
n-heptane	21	Table 23-2-(1.202)-vc API 44, Oct. 31, 1975
n-octane	18	H.L. Finke, M.E. Gross, G. Waddington and H.M. Huffman J Amer Chem Soc, 76, 333 (1954)
n-octane	13	T.J. Connelly, B.H. Sage and W.M. Lacey Ind and Eng Chem, 43, 4, 946 (1951) (smoothed data)
n-octane	5	H.M. Huffman, G.S. Parks and M. Barmore J Amer Chem Soc, 53, 3876 (1931)
n-octane	8	G.S. Parks, H.M. Huffman and S.B. Thomas J Amer Chem Soc, 52, 1032 (1930)
n-octane	6	Table 23-2-(1.203)-vc API 44, Oct. 31, 1976

n-nonane	22	H.L. Finke, M.E. Gross, G. Waddington and H.M. Huffman J Amer Chem Soc, 76, 333 (1954)
n-nonane	8	H.M. Huffman, G.S. Parks and M. Barmore J Amer Chem Soc, 53, 3876 (1931)
n-nonane	8	G.S. Parks, H.M. Huffman and S.B. Thomas J Amer Chem Soc, 52, 1032 (1930)
n-nonane	13	Table 23-2-(1.204)-vc API 44, Oct. 31, 1975
n-decane	17	H.L. Finke, M.E. Gross, G. Waddington and H.M. Huffman J Amer Chem Soc, 76, 333 (1954)
n-decane	6	H.M. Huffman, G.S. Parks and M. Barmore J Amer Chem Soc, 53, 3876 (1931)
n-decane	6	G.S. Parks, H.M. Huffman and S.B. Thomas J Amer Chem Soc, 52, 1032 (1930)
n-decane	10	Table 23-2-(1.205)-vc API 44, Oct. 31, 1976; Oct. 31, 1979
n-undecane	12	H.L. Finke, M.E. Gross, G. Waddington and H.M. Huffman J Amer Chem Soc, 76, 333 (1954)
n-undecane	5	H.M. Huffman, G.S. Parks and M. Barmore J Amer Chem Soc, 53, 3876 (1931)
n-dodecane	11	H.L. Finke, M.E. Gross, G. Waddington and H.M. Huffman J Amer Chem Soc, 76, 333 (1954)

n-dodecane	4	H.M. Huffman, G.S. Parks and M. Barmore J Amer Chem Soc, 53, 3876 (1931)
n-tridecane	8	H.L. Finke, M.E. Gross, G. Waddington and H.M. Huffman J Amer Chem Soc, 76, 333 (1954)
n-tetradecane	7	H.L. Finke, M.E. Gross, G. Waddington and H.M. Huffman J Amer Chem Soc, 76, 333 (1954)
n-pentadecane	7	H.L. Finke, M.E. Gross, G. Waddington and H.M. Huffman J Amer Chem Soc, 76, 333 (1954)
n-hexadecane	14	J.C. Petit and L.T. Minassian J Chem Thermo, 6, 1139 (1974)
n-hexadecane	9	H.L. Finke, M.E. Gross, G. Waddington and H.M. Huffman J Amer Chem Soc, 76, 333 (1954)
n-hexadecane	2	Parks, Moore, Renquist, Naylor, McClaine, Fujii and Hatton J Amer Chem Soc, 71, 3386 (1949)
n-heptadecane	11	J.F. Messerly, G.B. Guthrie, S.S. Todd and H.L. Finke J Chem and Eng Data, 12, 3, 338 (1967)
n-octadecane	11	J.F. Messerly, G.B. Guthrie, S.S. Todd and H.L. Finke J Chem and Eng Data, 12, 3, 338 (1967)
n-octadecane	1	G.S. Parks, G.E. Moore et al J Amer Chem Soc, 71, 3386 (1949)

n-pentacosane	5	M.E. Spaght, S.B. Thomas and G.S. Parks J Phys Chem, 36, 882 (1932)
n-hexacosane	10	R.J.L. Andon and J.F. Martin J Chem Thermo, 8, 1159 (1976)
isobutane	25	J.G. Aston, R.M. Kennedy and S.C. Schumann J Amer Chem Soc, 62, 2059 (1940)
isobutane	19	G.S. Parks, C.H. Shomate, W.D. Kennedy and B.L. Crawford Jr. J Chem Phys, 5, 359 (1937)
2-methylbutane	83	G.B. Guthrie jr and H.M. Huffman J Amer Chem Soc, 65, 1139 (1943)
2-methylbutane	14	G.S. Parks, H.M. Huffman and S.B. Thomas J Amer Chem Soc, 52, 1032 (1930)
2,2-dimethylpropane (neopentane)	3	H. Erokido, T. Shinoda and Y.-I. Mashiko Bull Chem Soc Jap, 42, 84 (1969)
2,2-dimethylpropane (neopentane)	4	J.G. Aston and G.H. Messerly J Amer Chem Soc, 58, 2354 (1936)
2-methylpentane	29	D.R. Doulsin and H.M. Huffman J Amer Chem Soc, 68, 1704 (1946)
2-methylpentane	22	Table 23-2-(1.201)-vc API 44, Oct. 31, 1975



3-methylpentane	21	D.R. Douslin and H.M. Huffman J Amer Chem Soc, 68, 1704 (1946)
3-methylpentane	24	H.L. Finke and J.F. Messerly J Chem Thermo, 5, 247 (1973)
3-methylpentane	24	Table 23-2-(1.201)-vc API 44, Oct. 31, 1975
2,3-dimethylbutane	38	D.R. Douslin and H.M. Huffman J Amer Chem Soc, 68, 1704 (1946)
2,3-dimethylbutane	19	Table 23-2-(1.201)-vc API 44, Oct. 31, 1975
2,2-dimethylbutane	17	D.R. Douslin and H.M. Huffman J Amer Chem Soc, 68, 1704 (1946)
2,2-dimethylbutane	15	Table 23-2-(1.201)-vc API 44, Oct. 31, 1975
2-methylhexane	19	H.M. Huffman, M.E. Gross, D.W. Scott and J.P. McCullough J Phys Chem, 65, 495 (1961)
2-methylhexane	12	G.S. Parks, H.M. Huffman and S.B. Thomas J Amer Chem Soc, 52, 1032 (1930)
2-methylhexane	17	Table 23-2-(1.202)-vc API 44, Oct. 31, 1975

3-methylhexane	10	H.M. Huffman, G.S. Parks and S.B. Thomas J Amer Chem Soc, 52, 3241, (1930)
2,2-dimethylpentane	20	H.M. Huffman, M.E. Gross, D.W. Scott and J.P. McCullough J Phys Chem, 65, 495 (1961)
2,2-dimethylpentane	14	H.M. Huffman, G.S. Parks and S.B. Thomas J Amer Chem Soc, 52, 3241 (1930)
2,2-dimethylpentane	19	Table 23-2-(1.202)-vc API 44, Oct. 31, 1975
2,3-dimethylpentane	69	H.L. Finke, J.F. Messerly and D.R. Douslin J Chem Thermo, 8, 965 (1976)
2,3-dimethylpentane	12	H.M. Huffman, G.S. Parks and S.B. Thomas J Amer Chem Soc, 52, 3241 (1930)
2,3-dimethylpentane	31	Table 23-2-(1.202)-vc API 44, Oct. 31, 1975
2,4,-dimethylpentane	40	H.M. Huffman, M.E. Gross, D.W. Scott and J.P. McCullough J Phys Chem, 65, 495 (1961)
2,4,-dimethylpentane	15	H.M. Huffman, G.S. Parks and S.B. Thomas J Amer Chem Soc, 52, 3241 (1930)
2,4,-dimethylpentane	18	Table 23-2-(1.202)-vc API 44, Oct. 31, 1975
3,3-dimethylpentane	28	H.L. Finke, J.F. Messerly and D.R. Douslin J Chem Thermo, 8, 965 (1976)

3,3-dimethylpentane	14	H.M. Huffman, G.S. Parks and S.B. Thomas J Amer Chem Soc, 52, 3241 (1930)
3,3-dimethylpentane	26	Table 23-2-(1.202)-vc API 44, Oct. 31, 1975
3-ethylpentane	46	H.M. Huffman, M.E. Gross, D.W. Scott and J.P. McCullough J Phys Chem, 65, 495 (1961)
3-ethylpentane	11	H.M. Huffman, G.S. Parks and S.B. Thomas J Amer Chem Soc, 52, 3241 (1930)
3-ethylpentane	17	Table 23-2-(1.202)-vc API 44, Oct. 31, 1975
2,2,3-trimethylbutane	10	H.M. Huffman, M.E. Gross, D.W. Scott and J.P. McCullough J Phys Chem, 65, 495 (1961)
2,2,3-trimethylbutane	6	H.M. Huffman, G.S. Parks and S.B. Thomas J Amer Chem Soc, 52, 3241 (1930)
2,2,3-trimethylbutane	10	Table 23-2-(1.202)-vc API 44, Oct. 31, 1975
2-methylheptane	4	E. Rajagopal and S.V. Subrahmanyam J Chem Thermo, 6, 873 (1974)
2-methylheptane	23	J.F. Messerly and H.L. Finke J Chem Thermo, 3, 675 (1971)
2-methylheptane	11	Table 23-2-(1.203)-vc API 44, Oct. 31, 1976

3-methylheptane	32	H.L. Finke and J.F. Messerly J Chem Thermo, 5, 247 (1973)
3-methylheptane	12	Table 23-2-(1.203)-vc API 44, Oct. 31, 1976
2,2,4-trimethylpentane	15	G.S. Parks, H.M. Huffman and S.B. Thomas J Amer Chem Soc, 52, 1032 (1930)
2,2,4-trimethylpentane	11	Table 23-2-(1.203)-vc API 44, Oct. 31, 1976
2,3,4-trimethylpentane	11	Table 23-2-(1.203)-vc API 44, Oct. 31, 1976
2,2,3,3-tetramethylbutane	3	D.W. Scott, D.R. Douslin, M.E. Gross, G.D. Oliver and H.M. Huffman J Amer Chem Soc, 74, 883 (1952)
2,2,3,3-tetramethylpentane	19	H.L. Finke, J.F. Messerly and D.R. Douslin J Chem Thermo, 8, 965 (1976)
2,2,3,3-tetramethylpentane	16	Table 23-2-(1.204)-vc API 44, Oct. 31, 1975
2,2,4,4-tetramethylpentane	19	H.L. Finke, J.F. Messerly and D.R. Douslin J Chem Thermo, 8, 965 (1976)
2,2,4,4-tetramethylpentane	20	Table 23-2-(1.204)-vc API 44, Oct. 31, 1975

3,3-diethylpentane	16	H.L. Finke, J.F. Messerly and D.R. Douslin J Chem Thermo, 8, 965 (1976)
3,3-diethylpentane	15	Table 23-2-(1.204)-vc API 44, Oct. 31, 1975
2-methylnonane	11	G.S. Parks, T.J. West and G.E. Moore J Amer Chem Soc, 63,1133 (1941) (smoothed data)
2-methylnonane	13	Table 23-2-(1.205)-vc API 44, Oct. 31, 1976; Oct. 31, 1979
3-methylnonane	12	G.S. Parks, T.J. West and G.E. Moore J Amer Chem Soc, 63, 1133 (1941) (smoothed data)
3-methylnonane	14	Table 23-2-(1.205)-vc API 44, Oct. 31, 1976; Oct. 31, 1979
4-methylnonane	13	G.S. Parks, T.J. West, G.E. Moore J Amer Chem Soc, 63, 1133 (1941) (smoothed data)
4-methylnonane	15	Table 23-2-(1.205)-vc API 44, Oct. 31, 1976; Oct. 31, 1979
5-methylnonane	12	G.S. Parks, T.J. West and G.E. Moore J Amer Chem Soc, 63, 1133 (1941) (smoothed data)
5-methylnonane	14	Table 23-2-(1.205)-vc API 44, Oct. 31, 1976; Oct. 31, 1979

2-methyldecane	22	J.F. Messerly and H.L. Finke J Chem Thermo, 3, 675 (1971)
cyclopentane	13	G.J. Szasz, J.A. Morrison, E.L. Pace and J.G. Aston J Chem Phys, 15, 8, 562 (1947) (smoothed data)
cyclopentane	16	D.R. Douslin and H.M. Huffman J Amer Chem Soc, 68, 173 (1946)
cyclohexane	9	J.L. San jose, G. Mellinger and R.C. Reid J Chem Eng Data, 21, 4, 414 (1976)
cyclohexane	4	J.G. Aston, G.J. Szasz and H.L. Finke J Amer Chem Soc, 65, 1135 (1943)
cyclohexane	7	R.A. Ruehrwein and H.M. Huffman J Amer Chem Soc, 65, 1620 (1943)
cyclohexane	5	G.S. Parks, H.M. Huffman and S.B. Thomas J Amer Chem Soc, 52, 1032 (1930)
cycloheptane	7	H.L. Finke, D.W. Scott, M.E. Gross, J.F. Messerly and G. Waddington J Amer Chem Soc, 78, 5469 (1956)
cyclooctane	6	H.L. Finke, D.W. Scott, M.E. Gross, J.F. Messerly and G. Waddington J Amer Chem Soc, 78, 5469 (1956)
bicyclohexyl (or cyclohexylcyclohexane)	44	D.F. O'Rourke and S.C. Mraw J Chem Thermo, 15, 489 (1983)

methylcyclopentane	13	T.J. Connolly, B.H. Sage and W.N. Lacey Ind and Eng Chem, 43, 4, 946 (1951) (smoothed data)
methylcyclopentane	32	D.R. Douslin and H.M. Huffman J Amer Chem Soc, 68, 173 (1946)
methylcyclopentane	8	H.M. Huffman, G.S. Parks and M. Barmore J Amer Chem Soc, 53, 3876 (1931)
ethylcyclopentane	21	M.E. Gross, G.D. Oliver and H.M. Huffman J Amer Chem Soc, 75, 2801 (1953)
1,1-dimethylcyclopentane	14	M.E. Gross, G.D. Oliver and H.M. Huffman J Amer Chem Soc, 75, 2801 (1953)
trans-1,2-dimethylcyclopentane	8	H.M. Huffman, G.S. Parks and M. Barmore J Amer Chem Soc, 53, 3876 (1931)
cis-1,2-dimethylcyclopentane	14	M.E. Gross, G.D. Oliver and H.M. Huffman J Amer Chem Soc, 75, 2801 (1953)
trans-1,3-dimethylcyclopentane	22	M.E. Gross, G.D. Oliver and H.M. Huffman J Amer Chem Soc, 75, 2801 (1953)
n-propylcyclopentane	25	J.F. Messerly, S.S. Todd and H.L. Finke J Phys Chem, 69, 353 (1965)

n-butylcyclopentane	24	J.F. Messerly, S.S. Todd and H.L. Finke J Phys Chem, 69, 353 (1965)
n-decylcyclopentane	12	J.F. Messerly, S.S. Todd and H.L. Finke J Phys Chem, 69, 353 (1965)
methylcyclohexane	15	D.R. Douslin and H.M. Huffman J Amer Chem Soc, 68, 173 (1946)
methylcyclohexane	12	G.S. Parks and H.M. Huffman J Amer Chem Soc, 52, 4381 (1930)
ethylcyclohexane	21	H.M. Huffman, S.S. Todd and G.D. Oliver J Amer Chem Soc, 71, 584 (1949)
ethylcyclohexane	15	Parks, Moore, Renquist, Naylor, McClaine, Fujii and Hatton J Amer Chem Soc, 71, 3386 (1949) (smoothed data)
1,1-dimethylcyclohexane	13	H.M. Huffman, S.S. Todd and G.D. Oliver J Amer Chem Soc, 71, 584 (1949)
cis-1,2-dimethylcyclohexane	16	H.M. Huffman, S.S. Todd and G.D. Oliver J Amer Chem Soc, 71, 584 (1949)
trans-1,2-dimethylcyclohexane	27	H.M. Huffman, S.S. Todd and G.D. Oliver J Amer Chem Soc, 71, 584 (1949)



cis-1,3-dimethylcyclohexane	18	H.M. Huffman, S.S. Todd and G.D. Oliver J Amer Chem Soc, 71, 584 (1949)
trans-1,3-dimethylcyclohexane	30	H.M. Huffman, S.S. Todd and G.D. Oliver J Amer Chem Soc, 71, 584 (1949)
cis-1,4-dimethylcyclohexane	22	H.M. Huffman, S.S. Todd and G.D. Oliver J Amer Chem Soc, 71, 584 (1949)
trans-1,4-dimethylcyclohexane	9	H.M. Huffman, S.S. Todd and G.D. Oliver J Amer Chem Soc, 71, 584 (1949)
n-propylcyclohexane	24	H.L. Finke, J.F. Messerly and S.S. Todd J Phys Chem, 69, 2094 (1965)
n-butylcyclohexane	21	H.L. Finke, J.F. Messerly and S.S. Todd J Phys Chem, 69, 2094 (1965)
n-heptylcyclohexane	7	Parks, Moore, Renquist, Naylor, McClaine, Fujii and Hatton J Amer Chem Soc, 71, 3386 (1949) (smoothed data)
n-decylcyclohexane	9	H.L. Finke, J.F. Messerly and S.S. Todd J Phys Chem, 69, 2094 (1965)
n-dodecylcyclohexane	2	Parks, Moore, Renquist, Naylor, McClaine, Fujii and Hatton J Amer Chem Soc, 71, 3386 (1949)

11-cyclohexylheneicosane	4	Parks, Moore, Renquist, Benjamin, Naylor, McClaine, Fujii and Hatton J Amer Chem Soc, 71, 3386 (1949)
cis-decalin	37	McCullough, Finke, Messerly, Todd, Kincheloe and Waddington J Phys Chem, 61, 1105 (1957)
trans-decalin	13	McCullough, Finke, Messerly, Todd, Kincheloe and Waddington J Phys Chem, 61, 1105 (1957)
benzene	6	J.L. San Jose, G. Mellinger and R.C. Reid J Chem Eng Data, 21, 4, 414 (1976) (smoothed data)
benzene	8	G.D. Oliver, M. Eaton and H.M. Huffman J Amer Chem Soc, 70, 1502 (1948)
benzene	6	H.M. Huffman, G.S. Parks and A.C. Daniels J Amer Chem Soc, 52, 1547 (1930)
benzene	11	Table 23-2-(33.1110)-vc API 44, Apr. 30, 1978
naphthalene	6	McCullough, Finke, Messerly, Todd, Kincheloe and Waddington J Phys Chem, 61, 1105 (1957)
naphthalene	11	M.E. Spaght, S.B. Thomas and G.S. Parks J Phys Chem, 36, 882 (1932)
anthracene	2	P. Goursot, H.L. Girdlar and E.F. Westrum J Phys Chem, 74, 12, 2538 (1970)

pyrene	7	W. Wong and E.F. Westrum, jr. J Chem Thermo, 3, 105 (1971)
toluene	8	P.T. Eubank, L.e cediell, J.C. Hoiste and K.R. Hall J Chem Eng Data, 29, 389 (1984)
toluene	8	J.L. San jose, G. Mellinger and R.C. Reid J Chem Eng Data, 21, 4, 414 (1976) (smoothed data)
toluene	24	Scott, Guthrie, Messerly, Todd, Berg, Hossenlopp and McCullough J Phys Chem, 66, 911 (1962)
toluene	23	Table 23-2-(33.1110)-vc API 44, Apr. 30, 1978
ethylbenzene	16	H.M. Huffman, G.S. Parks and A.C. Daniels J Amer Chem Soc, 52, 1547 (1930)
ethylbenzene	15	Table 23-2-(33.1110)-vc API 44, apr 30, 1978
o-xylene	8	H.M. Huffman, G.S. Parks and A.C. Daniels J Amer Chem Soc, 52, 1547 (1930)
o-xylene	8	Table 23-2-(33.1110)-vc API 44, Apr. 30, 1978
m-xylene	8	J.L. San Jose, G. Mellinger and R.C. Reid J Chem Eng Data, 21, 4, 414 (1976) (smoothed data)

m-xylene	6	H.M. Huffman, G.S. Parks and A.C. Daniels J Amer Chem Soc, 52, 1547 (1930)
m-xylene	11	Table 23-2-(33.1110)-vc API 44, Apr. 30, 1978
p-xylene	16	R.J. Corruccini and D.C. Ginnings J Amer Chem Soc, 69, 2291 (1947)
p-xylene	5	H.M. Huffman, G.S. Parks and A.C. Daniels J Amer Chem Soc, 52, 1547 (1930)
p-xylene	31	Table 23-2-(33.1110)-vc API 44, Apr. 30, 1978
n-propylbenzene	23	J.F. Messerly, S.S. Todd and H.L. Finke J Phys Chem, 69, 4304 (1965)
n-propylbenzene	22	Table 23-2-(33.1110)-vc API 44, Apr. 30, 1978
1,2,3-trimethylbenzene	25	R.D. Taylor, B.H. Johnson and J.E. Kilpatrick J Chem Phys, 23, 7, 1225 (1955)
1,2,3-trimethylbenzene	8	Table 23-2-(33.1110)-vc API 44, Apr. 30, 1978
1,2,4-trimethylbenzene	39	W.E. Putnam and J.E. Kilpatrick J Chem Phys, 27, 5, 1075 (1957)

1,2,4-trimethylbenzene	10	Table 23-2-(33.1110)-vc API 44, Apr. 30, 1978
1,3,5-trimethylbenzene	13	R.D. Taylor and J.E. Kilpatrick J Chem Phys, 23, 7, 1232 (1955)
1,3,5-trimethylbenzene	10	Table 23-2-(33.1110)-vc API 44, Apr. 30, 1978
diphenyl	3	M.E. Spaght, S.B. Thomas and G.S. Parks J Phys Chem, 36, 882 (1932)
diphenylmethane	4	H.M. Huffman, G.S.parks and A.C. Daniels J Amer Chem Soc, 52, 1547 (1930)
1,2-diphenylethane (or dibenzyl)	2	J.D. Ferry and S.B. Thomas J Phys Chem, 37, 253 (1933)
1-methylnaphthalene	15	McCullough, Finke, Messerly, Todd, Kincheloe and Waddington J Phys Chem, 61, 1105 (1957)
2-methylnaphthalene	9	McCullough, Finke, Messerly, Todd, Kincheloe and Waddington J Phys Chem, 61, 1105 (1957)
2-methylnaphthalene	1	H.M. Huffman, G.S. Parks and M. Barmore J Amer Chem Soc, 53, 3876 (1931)

1,2,3,4-tetrahydronaphthalene	11	McCullough, Finke, Messerly, Todd, Kincheloe and Waddington J Phys Chem, 61, 1105 (1957)
1,8-dimethylnaphthalene	7	H.L. Finke, J.F. Messerly, S.H. Lee, A.G. Osborn and D.R. Douslin J Chem Thermo, 9, 937 (1977)
2,6-dimethylnaphthalene	9	H.L. Finke, J.F. Messerly, S.H. Lee, A.G. Osborn and D.R. Douslin J Chem Thermo, 9, 937 (1977)
2,7-dimethylnaphthalene	6	H.L. Finke, J.F. Messerly, S.H. Lee, A.G. Osborn and D.R. Douslin J Chem Thermo, 9, 937 (1977)
phenanthrene	4	Finke, Messerly, Lee, Osborn and Douslin J Chem Thermo, 9, 937 (1977)
9,10-dihydrophenanthrene	34	S.H. Lee-Bechtold, I.A. Hossenlopp, D.W. Scott, A.G. Osborn and W.D. Good J Chem Thermo, 11, 469 (1979)
triphenylmethane	2	M.E. Spaght, S.B. Thomas and G.S. Parks J Phys Chem, 36, 882 (1932)
fluoranthene	5	W.-K. Wong and E.G. Westrum, Jr. J Chem Thermo, 3, 105 (1971)
1,2,3,4,5,6,7,8-octahydroanthracene	10	B.E. Gammon, J.E. Callanan, I.A. Hossenlopp, A.G. Osborn and W.D. Good presented at 8th Symposium on Thermophysical Properties, NBS, June 15-19

o-terphenyl	14	S.S. Chang and A.B. Bestul J Chem Phys, 56, 1, 503 (1972)
triphenylene	4	W. Wong and E.F. Westrum, jr. J Chem Thermo, 3, 105 (1971)
1,2'-dinaphthylmethane	10	H.L. Finke, J.F. Messerly, S.H. Lee, A.G. Osborn and D.R. Douslin J Chem Thermo, 9, 937 (1977)
n-butylbenzene	19	J.F. Messerly, S.S. Todd and H.L. Finke J Phys Chem, 69, 4304 (1965)
n-butylbenzene	8	H.M. Huffman, G.S. Parks and M. Barmore J Amer Chem Soc, 53, 3876 (1931)
tert-butylbenzene	8	H.M. Huffman, G.S. Parks and A.C. Daniels J Amer Chem Soc, 52, 1547 (1930)
1,2,4,5-tetramethylbenzene (or durene)	4	J.D. Ferry and S.B. Thomas J Phys Chem, 37, 253 (1933)
pentamethylbenzene	7	J.D. Ferry and S.B. Thomas J Phys Chem, 37, 253 (1933)
hexamethylbenzene	4	M.E. Spaght, S.B. Thomas and G.S. Parks J Phys Chem, 36, 882 (1932)

11-phenylheneicosane	1	Parks, Moore, Renquist, Naylor, McClaine, Fujii and Hatton J Amer Chem Soc, 71, 3386 (1949)
2,3-dihydroindene (or indan)	12	Table 23-2-(35.5200)-vc API 44, Apr. 30, 1983
1,1-dimethylindan	20	S.H. Lee-Bechtold, H.L. Finke, J.F. Messerly and D.W. Scott J Chem Thermo, 13, 213 (1981)
1,1-dimethylindan	20	Table 23-2-(35.5201)-vc API 44, Oct. 31, 1983
4,6-dimethylindan	12	S.H. Lee-Bechtold, H.L. Finke J.F. Messerly and D.W. Scott J Chem Thermo, 13, 213 (1981)
4,6-dimethylindan	15	Table 23-2-(35.5201)-vc API 44, Oct. 31, 1983
4,7-dimethylindan	11	S.H. Lee-Bechtold, H.L. Finke, J.F. Messerly and D.W. Scott J Chem Thermo, 13, 213 (1981)
4,7-dimethylindan	16	Table 23-2-(35.5201)-vc API 44, Oct. 31, 1983
1,1,4,6-tetramethylindan	12	S.H. Lee-Bechtold, H.L. Finke, J.F. Messerly and D.W. Scott J Chem Thermo, 13, 213 (1981)
1,1,4,7-tetramethylindan	20	S.H. Lee-Bechtold, H.L. Finke, J.F. Messerly and D.W. Scott J Chem Thermo, 13, 213 (1981)
fluorene	8	H.L. Finke, J.F. Messerly, S.H. Lee A.G. Osborn and D.R. Doustin J Chem Thermo, 9, 937 (1977)



TABLE A-2. LIQUID HEAT-CAPACITY DATA SOURCES FOR PURE HETEROATOMIC COMPOUNDS

COMPOUND	NUMBER	
	DATA PTS	DATA SOURCE
o-cresol	11	R.J.L. Andon, J.F. Counsell, E.B. Lees, J.F. Martin and C.J. Mash J Trans Faraday Soc, 63, 1115 (1967)
m-cresol	14	R.J.L. Andon, J.F. Counsell, E.B. Lees, J.F. Martin and C.J. Mash J Trans Faraday Soc, 63, 1115 (1967)
p-cresol	11	R.J.L. Andon, J.F. Counsell, E.B. Lees, J.F. Martin and C.J. Mash J Trans Faraday Soc, 63, 1115 (1967)
phenol	14	R.J.L. Andon, J.F. Counsell, E.F.G. Herington and J.F. Martin J Trans Faraday Soc, 59, 830 (1963)
furan	23	Guthrie, Scott, Hubbard, Katz, McCullough, Gross, Williamson and Waddington J Amer Chem Soc, 74, 4662 (1952)
o-dihydroxybenzene (catechol)	17	D.H. Andrews J Amer Chem Soc, 48, 1287 (1926)
m-dihydroxybenzene (resorcinol)	17	D.H. Andrews J Amer Chem Soc, 48, 1287 (1926)
p-dihydroxybenzene (hydroquinone)	17	D.H. Andrews J Amer Chem Soc, 48, 1287 (1926)

pyrrolidine	22	McCullough, Douslin, Hubbard, Todd, Messerly, Hossenlopp, Frow, Dawson and Waddington J Amer Chem Soc, 81, 5884 (1959)
pyrrole	20	Scott, Berg, Hossenlopp, Hubbard, Messerly, Todd, Douslin, McCullough, Waddington J Phys Chem, 71, 2263 (1967)
2-methylpyridine	19	Scott, Hubbard, Messerly, Todd, Hossenlopp, Good, Douslin and McCullough J Phys Chem, 67, 689 (1963)
pyridine	13	McCullough, Douslin, Messerly, Hossenlopp, Kincheloe and Waddington J Amer Chem Soc, 79, 4289 (1957)
aniline	3	G.S. Parks, H.M. Huffman and M. Barmore J Amer Chem Soc, 55, 2733 (1933)
aniline	11	E.W. Hough, D.M. Mason and B.H. Sage J Amer Chem Soc, 72, 5775 (1950)
dibenzothiophene	14	D.F. O'Rourke and S.C. Mraw J Chem Thermo, 15, 489 (1983)
cyclohexanethiol	21	J.F. Messerly, S.S. Todd and G.B. Guthrie, Jr. J Chem Eng Data, 12, 3, 426 (1967)
3-hexanethiol	25	McCullough, Finke, Hubbard, Todd, Messerly, Douslin and Waddington J Phys Chem, 65, 784 (1961)

3-methylthiophene	18	McCullough, Sunner, Finke, Hubbard, Gross, Pennington, Messerly, Good and Waddington J Amer Chem Soc, 75, 5075 (1953)
2-hexanethiol	23	McCullough, Finke, Hubbard, Todd, Messerly, Douslin and Waddington J Phys Chem, 65, 784 (1961)
1-hexanethiol	20	H.L. Finke, J.P. McCullough, J.F. Messerly, G.B. Guthrie and D.R. Douslin J Chem Thermo, 2, 27 (1970)
1-heptanethiol	16	H.L. Finke, J.P. McCullough, J.F. Messerly, G.B. Guthrie and D.R. Douslin J Chem Thermo, 2, 27 (1970)
1-decanethiol	30	H.L. Finke, J.P. McCullough, J.F. Messerly, G.B. Guthrie and D.R. Douslin J Chem Thermo, 2, 27 (1970)
3-pentanethiol	26	Scott, Finke, Hubbard, McCullough, Oliver, Gross, Katz, Williamson, and Waddington J Amer Chem Soc, 74, 4656 (1952)
2-pentanethiol	21	Scott, Finke, McCullough, Messerly, Pennington, Hossenlopp and Waddington J amer chem soc, 79, 1062 (1957)

## APPENDIX B

## ALTERNATE FORMS OF THE LIQUID HEAT-CAPACITY CORRELATION

For correlating heat capacities, several functional forms of the temperature variable were investigated; these included  $1/T$  and reduced temperatures,  $T/T^*$  and  $T/T_b$ , where  $T^*$  is a reducing temperature used in the perturbed-hard-chain equation of state;  $T_b$  is the normal boiling point in K.

Table B-1 summarizes the liquid-heat-capacity regression results for various forms of the temperature variable. Performance of the various forms, in terms of average deviation from experiment, were about equal.  $T$  was chosen as the temperature variable because it extrapolates to higher temperatures better than the other forms.

TABLE B-1. LIQUID HEAT-CAPACITY REGRESSION SUMMARY

Temperature Variable (a)	Number of		Percent Deviation	
	Compounds	Data Pts.	Average	Maximum
T	118	2969	2.3	12.0
1/T	118	2969	2.6	11.6
T/T*	33	962	1.9	7.2
T (b)	33	962	1.7	6.4
T/T <sub>b</sub>	111	2868	2.9	15.5
T (c)	111	2868	2.2	11.2

(a) Form of Heat-Capacity Correlation is:

$$C_p = A + B (\text{Temp. Var.}) + C (\text{Temp. Var.})^2$$

- (b) Using only data included in the T/T\* regression for comparison
- (c) Using only data included in the T/T<sub>b</sub> regression for comparison

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

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