Correlation of Liquid Heat Capacities for Carboxylic Esters

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Liquid heat capacity data of carboxylic esters (including a sebacate series, triglyceride series, and oligomer series), covering a temperature range from 20 to about 180 °C and a molecular weight range from 116 to 939, were determined with a differential scanning calorimeter. The data, together with published heat capacity values, were reduced to a temperature independent correlation. The results suggest an approximate additivity in carboxyl content and a lack of dependence on structural type (e.g., linear, branched, or oligomeric).

Liquid heat capacity is an important thermodynamic property of a substance and is useful in the description of the thermal motion of its molecules. Although carboxylic esters are used extensively in industrial applications (as solvents, plasticizers, etc.), few liquid heat capacity data exist as a function of temperature covering a wide molecular weight range. Estimation methods (*8*) for liquid heat capacity are generally available at or near 25 °C, and thus find limited use when applied to compounds having melting points greater than 25 °C. This paper reports the liquid heat capacity of a sebacate series, triglyceride series, and oligomer series obtained with a differential scanning calorimeter. These results, together with published data for alkanes and esters, were adequately correlated.

Experimental

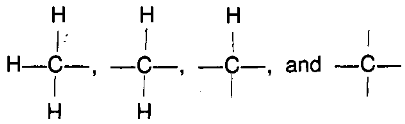
The compounds used are presented in Tables I, II, and IV–VII. The methods of preparation and characterization of the linear dialkyl sebacate esters (*4*), branched triglyceride esters (*4*), and oligomer esters of poly(hexamethylene sebacate) are available (*6, 7*). The liquid heat capacity data for the sebacates, triglycerides, and oligomer esters were obtained on the differential scanning calorimeter (DSC-1B, Perkin-Elmer) (*7*). Ten-milligram samples were sealed in aluminum pans and scanned at a rate of 10 °C/min over ranges of approximately 30 degrees. Scans were repeated for the reference and a standard 28.7-mg sapphire. The results were reproducible to about ±5%. The liquid heat capacity data for the simple esters and hydrocarbons were taken from the literature (*5, 9*).

Results

The liquid heat capacity of an ester molecule may be considered linear (*3, 7, 8*) in the number of alkane groups, N_i, and in the number of ester groups, N_{COO},

$$C_p(l) = \sum_{i=1}^{4} G_i(T)N_i + G_{\mathrm{COO}}(T, N_2)N_{\mathrm{COO}} \qquad (1)$$

where the sum in Equation 1 represents the contribution due to the alkane portion and $G_{\mathrm{COO}}(T, N_2)N_{\mathrm{COO}}$, that due to the ester groups [Symbols and notations are those used by Somayajalu and Zwolinski (*J. Chem. Soc. and Faraday Trans.*)]. For i = 1, 2, 3, and 4, the alkane groups are, respectively,



$$\mathrm{H{-}\overset{H}{\underset{H}{C}}{-}},\ \mathrm{{-}\overset{H}{\underset{H}{C}}{-}},\ \mathrm{{-}\overset{H}{\underset{|}{C}}{-}},\ \text{and}\ \mathrm{{-}\overset{|}{\underset{|}{C}}{-}}$$

For all of the compounds considered here, N_4 is zero. The temperature dependent coefficients for the alkane and carboxyl groups are, respectively, $G_i(T)$ and $G_{\mathrm{COO}}(T, N_2)$, where the latter is assumed to be also a function of N_2 (*7*). We will estimate the coefficients and then calculate $C_p(l)$ according to Equation 1.

Table I. Reduced Liquid Heat Capacity Data for n-Alkanes Used to Determine K_{12}, Ratio of Temperature Coefficients $G_1(T)$ to $G_2(T)$ [$C_p(l)$ Data Taken from Ref. *9*]

Formula	No. of temp values	Temp range, °C	$\left(\frac{\lambda_1}{N_1}\right)_{\mathrm{AV}}^a$
C_7H_{16}	33	−88.16–96.84	3.605 ± 0.072
C_8H_{18}	18	−50.55–24.42	4.049 ± 0.018
C_9H_{20}	22	−48.13–69.70	4.554 ± 0.028
$C_{10}H_{22}$	17	−26.14–45.46	5.042 ± 0.021
$C_{11}H_{24}$	12	−21.42–25.76	5.541 ± 0.018
$C_{12}H_{26}$	11	−6.47–44.25	6.044 ± 0.014
$C_{13}H_{28}$	8	−0.50–33.17	6.543 ± 0.011
$C_{14}H_{30}$	7	9.55–29.61	7.048 ± 0.003
$C_{15}H_{32}$	7	12.35–39.62	7.558 ± 0.009
$C_{16}H_{34}$	9	22.25–47.12	8.059 ± 0.008
$C_{25}H_{52}$	5	60–100	12.702 ± 0.085
$C_{33}H_{68}$	4	80–110	16.861 ± 0.029

[a] Average for the number of temperature values given with the standard error of estimate as the estimate of precision, where $\lambda_1 = C_p(l)/G_2(T)$.

Table II. Reduced Liquid Heat Capacity Data for Substituted n-Alkanes Used to Determine K_{32}, Ratio of Temperature Coefficients $G_3(T)$ to $G_2(T)$ [$C_p(l)$ Data Taken from Ref. *9*]

Compound	No. of temp values	Temp range, °C	$\left(\frac{\lambda_3}{N_3}\right)_{\mathrm{AV}}^a$
2,4-Dimethylpentane	40	−112.34–33.94	1.372 ± 0.135
2,3-Dimethylhexane	3	124.34–249.04	1.657 ± 0.162
3,4-Dimethylhexane	3	133.54–249.44	1.666 ± 0.148
2-Methylhexane	19	−112.74–28.02	3.866 ± 0.129
3-Ethylpentane	46	−127.96–25.64	3.706 ± 0.156
3-Ethylhexane	3	123.94–249.54	4.313 ± 0.294

[a] Average for the number of temperature values given with the standard error of estimate as the estimate of precision, where $\lambda_3 = [C_p(l)/G_2(T)] - K_{12}N_1$.

The molecular weight of the ester molecule may be represented as

$$M = \sum_{i=1}^{4} W_i N_i + W_{\text{coo}} N_{\text{coo}} \tag{2}$$

where W_i and W_{coo} are the respective weights of the alkane groups and carboxyl group (i.e., $W_1 = 15.0$, $W_2 = 14.0$, $W_3 = 13.0$, $W_4 = 12.0$, and $W_{\text{coo}} = 44.0$).

Temperature dependent coefficients for alkane groups. Only the coefficients for i = 1, 2, and 3 will be considered here ($N_4 = 0$). The coefficient, $G_2(T)$, has been estimated from n-alkane data by Broadhurst (*1*) as

$$G_2(T) = 0.00818\,T + 5.00 \tag{3}$$

where T is the absolute temperature and the units are calories per degree per mole. By expanding the sum in Equation 1 and setting $N_{\text{coo}} = 0$, Equation 1 becomes

$$C_p(l) = G_1(T)N_1 + G_2(T)N_2 + G_3(T)N_3 \tag{4}$$

Table III. Estimated Values for Ratios K_{12} and K_{32} Determined According to Equations 5 and 6

Ratio	Estd value
K_{12}	1.03
K_{32}	0.80

For the case of n-alkanes ($N_3 = 0$), Equation 4 may be rearranged to the following reduced form:

$$\frac{\lambda_1}{N_1} = \frac{C_p(l)/G_2(T)}{N_1} = \frac{N_2}{N_1} + K_{12} \tag{5}$$

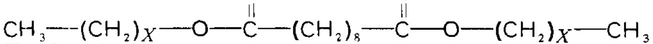
where $\lambda_1 = C_p(l)/G_2(T)$ is assumed temperature independent, and the ratio $K_{12} = G_1(T)/G_2(T)$ is assumed to be constant. Using the results of Equation 5, Equation 4 may be rearranged again as follows:

$$\frac{\lambda_3}{N_3} = \frac{[C_p(l)/G_2(T)] - K_{12}N_1}{N_3} = \frac{N_2}{N_3} + K_{32} \tag{6}$$

where $\lambda_3 = [C_p(l)/G_2(T)] - K_{12}N_1$ is also assumed to be temperature independent, and the ratio $K_{32} = G_3(T)/G_2(T)$ is assumed to be constant. Alkane data from Timmermans (*9*), which are summarized in Tables I and II, were used to evaluate the constants in Equations 5 and 6. The constant K_{12} was first estimated from n-alkane data by plotting $(\lambda_1/N_1)_{\text{AV}}$ vs. N_2/N_1, and the constant K_{32} was estimated from a plot of $(\lambda_3/N_3)_{\text{AV}}$ vs. N_2/N_3 by using Equation 6. Hence, the estimated coefficients are given, respectively, as $G_1(T) = K_{12}G_2(T)$ and $G_3(T) = K_{32}G_2(T)$. The estimated values for K_{12} and K_{32} are given in Table III.

Temperature dependent coefficient for carboxyl group. From a development analogous to that used for Equations 5 and 6, the reduced expression for the carboxyl group is given as

Table IV. Liquid Heat Capacity, $C_p(l)$, at Various Temperatures of Linear Esters of Sebacic Series



$$CH_3{-}(CH_2)_X{-}O{-}\overset{\overset{\large O}{\|}}{C}{-}(CH_2)_8{-}\overset{\overset{\large O}{\|}}{C}{-}O{-}(CH_2)_X{-}CH_3$$

$X = 3 - 17$

Compound	Empirical formula	MW	Liquid heat capacity, cal/deg mol						$\left(\frac{\lambda_{\text{coo}}}{N_{\text{coo}}}\right)^a_{\text{AV}}$
Di-n-butyl sebacate	$C_{18}H_{34}O_4$	314.45	T, K:	312	337	362	387	412	9.08 ± 0.58
			C_p, exptl:	148	152	163	164	179	
			C_p, calcd:	150	154	158	162	167	
			% Dev:	−1.4	−1.3	3.1	1.2	6.7	
Di-n-hexyl sebacate	$C_{22}H_{42}O_4$	370.34	T, K:	315	340	365	390	414	10.94 ± 0.48
			C_p, exptl:	175	177	198	201	206	
			C_p, calcd:	179	184	189	194	199	
			% Dev:	−2.3	−4.0	4.6	3.5	3.4	
Di-n-octyl sebacate	$C_{26}H_{50}O_4$	426.00	T, K:	318	343	368	393		12.24 ± 0.11
			C_p, exptl:	203	208	210	219		
			C_p, calcd:	209	214	220	225		
			% Dev:	−3.0	−2.9	−4.8	−2.7		
Di-n-decyl sebacate	$C_{30}H_{58}O_4$	482.79	T, K:	368	393	403			14.40 ± 0.54
			C_p, exptl:	240	251	266			
			C_p, calcd:	250	256	259			
			% Dev:	−4.2	−2.0	2.6			
Di-n-dodecyl sebacate	$C_{34}H_{66}O_4$	539.00	T, K:	368	398	408			15.98 ± 0.32
			C_p, exptl:	267	283	288			
			C_p, calcd:	280	289	292			
			% Dev:	−4.9	−2.1	−1.4			
Di-n-tetra decyl sebacate	$C_{38}H_{74}O_4$	595.00	T, K:	343	353	378	418	433	18.70 ± 0.46
			C_p, exptl:	298	308	321	342	340	
			C_p, calcd:	303	306	314	327	332	
			% Dev:	−1.7	0.65	2.2	4.4	2.4	
Di-n-hexa decyl sebacate	$C_{42}H_{82}O_4$	651.36	T, K:	353	368	378	418		21.09 ± 0.49
			C_p, exptl:	349	347	355	384		
			C_p, calcd:	336	341	348	350		
			% Dev:	3.7	1.7	2.0	6.5		
Di-n-octa decyl sebacate	$C_{46}H_{90}O_4$	707.36	T, K:	353	368	378	403	453	21.18 ± 0.76
			C_p, exptl:	354	374	357	365	370	
			C_p, calcd:	366	372	376	385	404	
			% Dev:	−3.4	0.54	−5.5	−5.5	−9.2	
Average error		3.3%							
Standard error of estimate		1.9							

[a] Average for the temperatures given with the standard error of estimate as the estimate of precision, where $\lambda_{\text{coo}} = C_p(l)/G_2(T) - K_{12}N_1$.

$$\frac{\lambda_{coo}}{N_{coo}} = \frac{N_2}{N_{coo}} + K_{coo} \tag{7}$$

where λ_{coo} is also assumed to be temperature independent, and K_{coo}, the ratio of $G_{coo}(T, N_2)$ to $G_2(T)$, according to Equation 1 is assumed to be dependent on the number of methylene groups, N_2. The lambda function for the carboxyl group ($N_4 = 0$) is given as

$$\lambda_{coo} = C_p(l)/G_2(T) - [K_{12}N_1 + K_{32}N_3] \tag{8}$$

From data in Tables IV–VII and the use of Equation 7, the ratio of coefficients was empirically separated as a function of N_2 to yield

$$K_{coo} = F(N_2) + c = \frac{-0.025\ N_2 + 1.40}{1 + 0.00015(N_2)^2} + 0.90 \tag{9}$$

where the form of $F(N_2)$ was chosen only to best represent the data. Therefore, Equation 7 with $N_4 = 0$ may be rewritten as

$$\lambda'_{coo} = \frac{\lambda_{coo}}{N_{coo}} - F(N_2) = \frac{N_2}{N_{coo}} + 0.90 \tag{10}$$

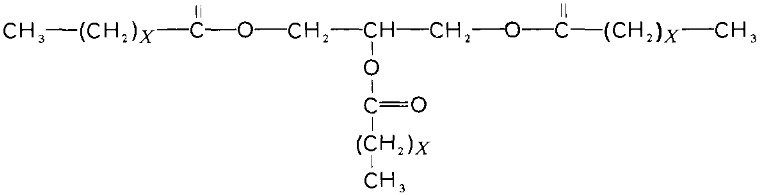
In Figure 1 we show a plot of λ'_{coo} vs. N_2/N_{coo}. The solid line was drawn according to Equation 10 with a slope of 1 and an intercept of 0.90. From Equations 8–10, the liquid heat capacity in calories per degree per mole is given as

$$C_p(l) = \left[\left(\frac{N_2}{N_{coo}} + K_{coo}\right) N_{coo} + K_{12}N_1 + K_{32}N_3\right] G_2(T) \tag{11}$$

The procedure for utilizing Equation 11 may be shown from a typical calculation. For example, diethyl succinate ($CH_3CH_2OOCCH_2CH_2COOCH_2CH_3$): $N_1 = 2$; $N_2 = 4$; $N_3 = 0$; $N_{coo} = 2$; $G_2(293.15\ K) = 7.398$; $K_{12} = 1.03$; $F(N_2) = 1.30$; $K_{coo} = 2.20$; therefore, $C_p(l) = [(4/2 + 2.20) \times 2 + (1.03 \times 2)] \times 7.398 = 77.3$ (deviation = 2.23%). The data in Tables IV–VII were calculated using Equation 11 with an average error of 2.5%, the average standard estimate of error being 1.7. Thus, the correlation of Equation 10 reasonably represents the data in this study.

By solving Equation 2 for N_2 and inserting the results into Equation 1, the simplified expression ($N_4 = 0$) in calories per degree per mole becomes

Table V. Liquid Heat Capacity, $C_p(l)$, at Various Temperatures of Branched Esters of Triglyceride Series



$X = 2 - 16$

Compound	Empirical formula	MW	Liquid heat capacity, cal/deg mol						$\left(\frac{\lambda_{coo}}{N_{coo}}\right)_{AV}^{a}$
Tributyrin	$C_{15}H_{26}O_6$	302.37	T, K:	313	338	363	388	413	4.87 ± 0.18
			C_p, exptl:	136	148	145	150	161	
			C_p, calcd:	137	141	145	148	152	
			% Dev:	−0.74	4.7	0.0	1.3	5.6	
Tricaproin	$C_{21}H_{38}O_6$	386.50	T, K:	313	338	363	388	413	6.67 ± 0.23
			C_p, exptl:	180	179	196	195	204	
			C_p, calcd:	179	184	188	193	198	
			% Dev:	0.56	−2.8	4.1	1.0	2.9	
Trioctanoin	$C_{27}H_{50}O_6$	470.69	T, K:	338	388	413			8.12 ± 0.12
			C_p, exptl:	220	234	234			
			C_p, calcd:	226	238	244			
			% Dev:	−2.7	−1.7	−4.3			
Tridecanoin	$C_{33}H_{62}O_6$	554.86	T, K:	313	363	388			10.39 ± 0.17
			C_p, exptl:	265	284	283			
			C_p, calcd:	262	276	283			
			% Dev:	1.1	2.8	0.0			
Trilaurin	$C_{39}H_{74}O_6$	639.02	T, K:	323	348	373	398		13.92 ± 0.52
			C_p, exptl:	312	309	326	333		
			C_p, calcd:	307	315	323	332		
			% Dev:	1.6	−1.9	0.92	0.30		
Trimyristin	$C_{45}H_{86}O_6$	723.18	T, K:	333	358	383	408	433	13.92 ± 0.52
			C_p, exptl:	354	365	387	382	369	
			C_p, calcd:	353	362	372	381	390	
			% Dev:	0.28	0.82	3.9	0.26	−5.7	
Tripalmitin	$C_{51}H_{98}O_6$	807.34	T, K:	343	368	393	418		16.07 ± 0.55
			C_p, exptl:	398	413	445	452		
			C_p, calcd:	400	411	421	432		
			% Dev:	−0.50	0.48	5.4	4.4		
Tristearin	$C_{57}H_{110}O_6$	890.50	T, K:	353	378	403	428	453	18.55 ± 0.42
			C_p, exptl:	472	498	494	494	513	
			C_p, calcd:	449	461	472	484	496	
			% Dev:	4.9	7.4	4.4	2.0	3.3	

Average error 2.5%
Standard error of estimate 2.0

[a] Average for the temperatures given with the standard error of estimate as the estimate of precision, where $\lambda_{coo} = C_p(l)/G_2(T) - [K_{12}N_1 + K_{32}N_3]$.

$$C_p(l) = [G_2(T)/W_2]M + \Delta_{\mathrm{coo}}N_{\mathrm{coo}} + \Delta_1N_1 + \Delta_3N_3 \quad (12)$$

where for the alkanes, $\Delta_j = G_j(T) - [G_2(T)/W_2]W_j$, $j = 1$ and 3; and for the carboxyl group, $\Delta_{\mathrm{coo}} = G_{\mathrm{coo}}(T, N_2) - [G_2(T)/W_2]W_{\mathrm{coo}}$.

The results shown in Figure 2 at 20 °C ($N_4 = 0$) were calculated from Equation 12. The plot shows that the effect of carboxyl addition to an alkane chain is to reduce the heat capacity proportionally to the number of carboxyl groups in the chain. If the heat capacity depends on both molecular weight and carboxyl content, then an oligomeric series is formed as shown by the dotted line in Figure 2. By transforming Equation 12 to calories per degree per gram (by dividing both sides of the equation by M), one may examine the limiting value for an oligomer series at infinite chain length (molecular weight goes to infinity), i.e.,

$$\lim_{M\to\infty} C_p(l)/M = G_2(T)/W_2 + [c - W_{\mathrm{coo}}/W_2]G_2(T) \lim_{M\to\infty} N_{\mathrm{coo}}/M \quad (13)$$

Equation 13 allows a rough estimate of flexibility effects (*2*) for esters in the polymer regime. For example, Equation 13 predicts at 20 °C for the oligomers of this study a limiting value of 0.42 vs. a value of 0.53 for the *n*-alkanes.

Conclusions

The results presented here allow an easy estimation of liquid heat capacity to about 3% for carboxylic esters as a function of temperature and molecular weight where only N_2, N_{coo}, and the alkane groups, (i.e., N_1 and N_3) must be known; the type of structure is unimportant if the correlation of Equation 10 is used. A variation of 5% in $\lambda_{\mathrm{coo}}/N_{\mathrm{coo}}$ causes the calculated heat capacity to vary about 5%. Hence, the error estimate of $\lambda_{\mathrm{coo}}/N_{\mathrm{coo}}$ in Tables IV–VI is within the error of the experimental values of $C_p(l)$.

Acknowledgment

The authors express their appreciation to the National Bureau of Standards for the use of its facilities.

Table VI. Liquid Heat Capacity, $C_p(l)$, at Various Temperatures of Linear Oligomer Esters of Poly(hexamethylene sebacate)
$CH_3{-}(CH_2)_5{-}OOC{-}(CH_2)_8{-}COO{-}[(CH_2)_6{-}OOC{-}(CH_2)_8{-}COO]_{X\text{-}1}{-}(CH_2)_5{-}CH_3$
$X = 1, 2, 3, \ldots$

X	Empirical formula	MW		Liquid heat capacity, cal/deg mol							$\left(\frac{\lambda_{\mathrm{coo}}}{N_{\mathrm{coo}}}\right)^a_{\mathrm{AV}}$
1	$C_{22}H_{42}O_4$	370.34	T, K:	303	313	323	343	373	383	393	10.70 ± 0.42
			C_p, exptl:	170	171	173	182	195	199	200	
			C_p, calcd:	177	179	181	185	191	192	194	
			% Dev:	−4.1	−4.7	−4.5	−1.6	2.0	3.5	3.0	
2	$C_{38}H_{70}O_8$	654.56	T, K:	328	365	388	408				9.42 ± 0.09
			C_p, exptl:	309	316	322	331				
			C_p, calcd:	305	317	325	331				
			% Dev:	1.3	−0.32	−0.93	0.0				
3	$C_{54}H_{98}O_{12}$	938.78	T, K:	333	373	413	433				8.76 ± 0.24
			C_p, exptl:	437	442	451	455				
			C_p, calcd:	422	440	458	466				
			% Dev:	3.4	0.45	−1.6	−2.4				

Average error 2.3%
Standard error of estimate 1.6

[a] Average for the temperatures given with the standard error of estimate as the estimate of precision, where $\lambda_{\mathrm{coo}} = C_p(l)/G_2(T) - K_{12}N_1$.

Table VII. Liquid Heat Capacity, $C_p(l)$, at 293.15 K of Carboxylic Esters (Data Taken from Ref. *5*)

		Liquid heat capacity, cal/deg mol			
Compound	MW	Exptl	Calcd	% Dev	$\left(\frac{\lambda_{\mathrm{coo}}}{N_{\mathrm{coo}}}\right)^a$
i-Butyl acetate	116.1	53.3	53.9	−1.13	5.14
Ethyl valerate	130.2	59.8	61.1	−2.17	6.02
Propyl valerate	144.2	66.2	68.3	−3.17	6.88
Diethyl oxalate	146.1	63.3	63.3	0.00	3.25
Butyl valerate	158.2	72.6	75.5	−3.99	7.75
Diethyl malonate	160.1	69.3	70.3	−1.44	3.65
Diethyl succinate	174.9	79.06	77.3	2.23	4.31
Dibutyl oxalate	202.2	89.2	91.3	−2.35	5.00
Diisoamyl oxalate	230.3	103.4	105.3	−1.84	5.96

Average error 2.04%
Standard error of estimate 1.15

[a] $\lambda_{\mathrm{coo}} = C_p(l)/G_2(T) - K_{12}N_1$.

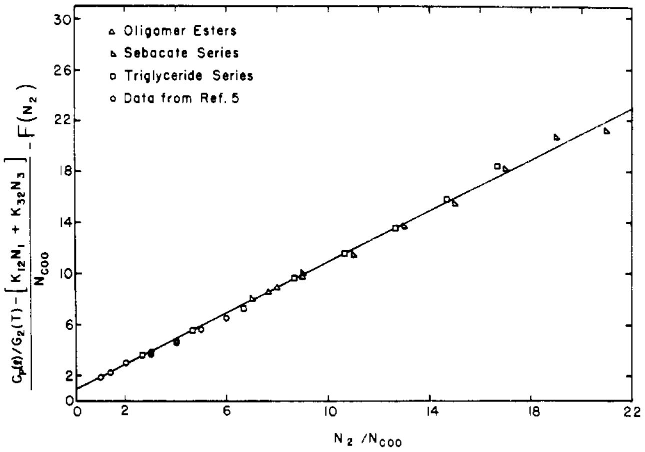


Figure 1. Reduced liquid heat capacities, λ'_{coo}, of carboxylic esters vs. ratio of methylene groups to carboxyl groups (N_2/N_{coo}). Solid line calculated according to Equation 10

Nomenclature

c = empirical constant

$C_p(l)$ = liquid heat capacity

Δ_{coo} = $G_{coo}(T, N_2) - [G_2(T)/W_2]\, W_{coo}$

Δ_j = $G_j(T) - [G_2(T)/W_2]\, W_j$; j = 1, 3, and 4

$F(N_2)$ = empirical function of number of methylene groups

$G_{coo}(T, N_2)$ = temperature dependent coefficient of the carboxyl group (as a function of N_2)

$G_j(T)$ = temperature dependent coefficient of alkane groups; j = 1, 2, 3, 4

j = alkane groups (1 = CH_3; 2 = CH_2; 3 = CH; 4 = C)

K_{coo} = $G_{coo}(T, N_2)/G_2(T) = F(N_2) + c$ = ratio of coefficient of carboxyl group to that of coefficient of methylene group

K_{j2} = $G_j(T)/G_2(T)$ = ratio of coefficient of j group to that of coefficient of methylene group; j = 1, 3, and 4

λ_{coo} = temperature independent function of carboxyl group

λ_j = temperature independent function of alkane groups; j = 1, 3, and 4

N_{coo} = number of carboxyl group per molecule

N_j = number of alkane groups per molecule; j = 1, 2, 3, 4

W_{coo} = molecular weight of carboxyl group

W_j = molecular weight of alkane groups; j = 1, 2, 3, 4

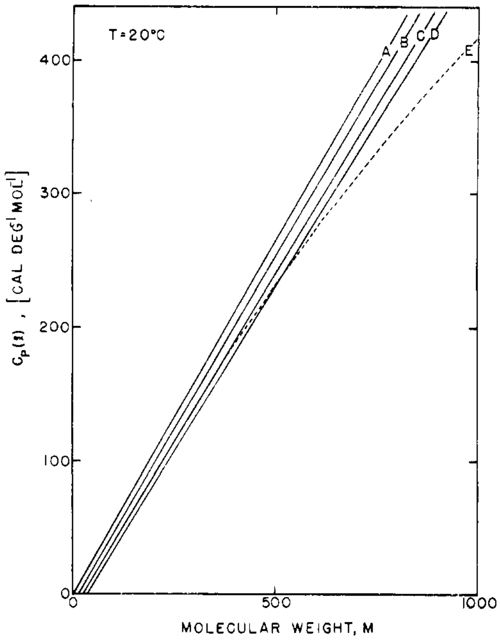


Figure 2. Calculated liquid heat capacities according to Equation 12 vs. molecular weight: A, N_{coo} = 0 (n-alkanes); B, N_{coo} = 1 (monocarboxylics); C, N_{coo} = 2 (dicarboxylics and sebacates); D, N_{coo} = 3 (triglycerides); E, N_{coo} = 2, 4, 6, . . . (oligomers)

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