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A correlation of latent heats and densities of pure organic liquids from known vapor pressure data

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A CORRELATION OF LATENT HEATS AND DENSITIES OF PURE ORGANIC LIQUIDS FROM KNOWN VAPOR PRESSURE DATA

by

VINCENT J. VASTA, JR.

A THESIS

PRESENTED IN PARTIAL FULFILLMENT OF

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Abstract

Employing the correlation developed by Kemme (5), which is based on a hole model for a liquid, relating vapor pressures with corresponding liquid densities and the number of carbon atoms in a molecular chain for a homologous series, correlation coefficients were established using multi-linear regression analysis on available literature data. This correlation was newly applied to several straight chain homologous series including the n-acids, formate esters and n-alkyl benzenes.

A second correlation developed by Kemme (5) relating vapor pressure, internal heat of vaporization and the number of carbon atoms for a homologous series was employed to determine correlation coefficients for several series of normal straight chain hydrocarbons not considered by Kemme. This correlation was applied to the n-alcohols, n-alkyl-chlorides, n-acids, formate esters and n-alkyl benzenes. This correlation was also used to determine internal heats of vaporization at pressures above 760 mm. Hg. for the n-alkyl benzenes.

This correlation was also used to compare the energies of vaporization attributable to the various functional groups, independent of the rest of the molecule.

APPROVAL OF THESIS

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I would like to express my appreciation to Dr. Saul I. Kreps for his continued assistance and thoughtful review of this work. His guidance and concern were invaluable assets without which this work would not have been completed.

I would also like to thank my wife, Ginny, for her understanding, patience and skilled assistance in typing this manuscript.

V. J. V.

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Introduction

Kemme (5) discussed the relationships existing between vapor pressure and other physical and thermodynamic properties of pure organic liquids. He concluded that it would be quite desirable to relate vapor pressure to other properties in that, since vapor pressure is one of the more variable properties, reasonably accurate vapor pressure data could be used to predict unknown properties with relative confidence.

The desirability of such relationships becomes apparent when one considers its applicability in electronic data processing. Such relationships could be easily stored in memory in place of a vast array of individual pieces of data. The savings in computer memory space that this would afford could be quite significant.

The purpose of this work is to further investigate some of the "inter-property" relationships considered by Kemme. Employing the correlations developed by Kemme investigations were conducted both with regard to the relationship between vapor pressure and liquid densities and that between vapor pressure and internal heat of vaporization.

As with Kemme's investigations, this study concerns itself only with normal straight chain homologous series, in order that the effects of structure can be more easily defined. The series

considered were dictated by the availability of adequate literature data to yield significant results. The data used are presented in the appendix. For the density correlation the following series were considered: n-acids, formate esters, and n-alkyl benzenes. For the internal heat of vaporization correlation the following series were investigated: n-alcohols, n-alkyl chlorides, n-acids, formate esters and n-alkyl benzenes.

INTRODUCTION TO LIQUID STATE THEORY

Kemme (5) gives an excellent treatment of the aspects of liquid state theory which should be known in order to understand the theoretical derivations which follow in the next section. I will attempt here only to highlight some of the more essential points in this treatment.

Liquid Models

It is convenient to assume a model for the liquid state in order to relate the physical properties of a liquid by theoretically derivable considerations. Several models are available e.g. cell, hole and tunnel models, however, due to its relative simplicity, the hole model was selected by Kemme to describe a system of large regular molecules.

A Hole Theory of Liquids

The hole theory of liquids requires that a liquid system be divided into an array of constant size cells which is invariant with temperature and pressure. The size of the cell must be such that simultaneous entry of two molecules into one cell can be neglected due to the repulsive forces between molecules. A given liquid state consists of a system of cells, some of which are full and others empty. As the temperature of this liquid increases,

the number of empty cells increases, resulting in an increase in volume and a corresponding decrease in density.

In considering any long chain molecule a cell volume, τ, may be chosen which is independent of the chain length and which occupies a volume somewhat larger than a methane molecule. A given molecule containing n carbon atoms would therefore occupy a certain number of consecutive cells, x.

Kurata and Isida (6) applied the hole model to normal paraffin liquids in order to relate the number of carbon atoms in a molecular chain with the normal boiling point, critical properties and heat of vaporization at atmospheric pressure. Their development is used as a basis for an equation which relates liquid density with vapor pressure and the number of carbon atoms. It also leads to a second equation which relates the heat of vaporization with vapor pressure and the number of carbon atoms.

The Kurata-Isida Vapor Pressure Equation

Starting with the equation for total free energy as developed by Kemme (5).

$$F = N_o f + kT\left[\left\{ v/\tau - xN_o \right\} \ln \left\{ 1-(\tau xN_o/v) \right\} + N_o \ln(\tau xN_o/v) \right]$$

$$+(z\psi/2)\ (v - \tau x\ N_o)\ (x\ N_o/v) \qquad (1)$$

The following is the derivation of Kurata-Isida (6). The pressure P, and chemical potential μ, of a system may be described by

$$P = -\left(\frac{\delta F}{\delta v}\right)_{T,N} \qquad (2)$$

$$= \left(\frac{\delta F}{\delta N_o}\right)_{T,v} \qquad (3)$$

Differentiating equation (1) as per equations (2) and (3) yields

$$P= -\left(\frac{\delta F}{\delta v}\right)_{T,N} = -\frac{kT}{\tau}\left[\ln\left\{1 - \frac{\tau xN_o}{v}\right\} + (v-xN_o\tau)\left(\frac{\tau xN_o}{v^2}\right)\left(\frac{v}{v-\tau xN_o}\right)\right.$$

$$\left. + \left(\frac{-\tau N_o}{v}\right)\right] - \left(\frac{z\psi}{2\tau}\right)\left(\frac{\tau xN_o}{v}\right)^2 \qquad (4)$$

and

$$\mu = \left(\frac{\delta F}{\delta N_o}\right)_{T,v} = f + kT\left[\left(\frac{v}{\tau} - xN_o\right)\left(\frac{-\tau x}{v - \tau N_o}\right) - x\ln\left(1 - \frac{\tau x N_o}{v}\right) + 1\right.$$

$$\left. + \ln\left(\tau x \frac{N}{v}\right)\right] + \frac{xz\psi}{2}\left[1 - \frac{2\tau x N_o}{v}\right] \qquad (5)$$

Rearranging equations (4) and (5) and substituting v, the volume per molecule, for v/N_o, yields

$$P = -\frac{kT}{\tau}\left\{\ln\left(1 - \frac{x\tau}{v}\right) + (x-1)\,\tau/v\right\} - \frac{z\psi}{2\tau}\left(\frac{x\tau}{v}\right)^2 \qquad (6)$$

$$\mu = f + kT\left\{\ln\left(\frac{xT}{v}\right) - x\ln\left(1 - \frac{x\tau}{v}\right) - (x-1)\right\}$$

$$+ \frac{z x \psi}{2}\left(1 - \frac{2x\tau}{v}\right) \qquad (7)$$

For a two phase system to be at equilibrium the pressures and the chemical potentials of the two phases must be equal such that

$$P_g = P_l$$

and

$$\mu_g = \mu_l$$

The subscripts g and l represent the gas and liquid phase respectively. Therefore one may write:

$$\ln\left(1 - \frac{x\tau}{v_g}\right) + (x-1)\frac{\tau}{v_g} + \frac{z\psi}{2kT}\left(\frac{x\tau}{v_g}\right)^2 = \ln\left(1 - \frac{x\tau}{v_l}\right) + (x-1)\frac{\tau}{v_l}$$

$$+ \frac{z\psi}{2kT}\left(\frac{x\tau}{v_l}\right)^2 \qquad (8)$$

and

$$\frac{1}{x}\ln\left(\frac{x\tau}{v_g}\right) - \ln\left(1-\frac{x\tau}{v_g}\right) + \frac{g\psi}{2kT}\left(1-\frac{2x\tau}{v_g}\right) =$$

$$\frac{1}{x}\ln\left(\frac{x\tau}{v_l}\right) - \ln\left(1-\frac{x\tau}{v_l}\right) + \frac{g\psi}{2kT}\left(1-\frac{2x\tau}{v_l}\right) \qquad (9)$$

assuming

$$f_l = f_g$$

If we assume for simplicity that v_g is very large compared with v_l or $x\tau$ at temperatures below the boiling point, equation (6) then reduces to the ideal gas equation

$$P = \frac{kT}{v_g} \qquad (10)$$

When equations (8) and (9) are combined with equation (10) and assuming v_g much greater than v_l one gets,

$$\ln P = \ln\left(\frac{kT}{v_l}\right) + (x-1)\left(\frac{x\tau}{v_l}\right) - \frac{xg\psi}{2kT}\left(\frac{x\tau}{v_l}\right)\left(2-\frac{x\tau}{v_l}\right) \qquad (11)$$

This is the Kurata-Isida vapor pressure equation.

The Kurata-Isida Heat of Vaporization Equation

Starting with equation (11) and assuming that $x\gamma = v_1$ and noting that $\psi = \epsilon - Ts$, Kurata and Isida (6) obtained:

$$\ln P = \ln\left({}^{kT}/_{x\gamma}\right) + x\left\{1\left({}^{zs}/_{2k}\right)\right\} - 1 - x\left({}^{z\epsilon}/_{2kT}\right) \qquad (12)$$

where ϵ and s are the internal energy and entropy terms respectively, which are associated with the Helmholtz free energy change, ψ. Assuming for simplicity that ϵ and s are independent of temperature, so that equation (12) could be simply differentiated, and realizing that $R = N_A k$ the following result was obtained:

$$\frac{dP}{dT} = \frac{P}{T} + \frac{P}{T^2}\left(\frac{N_A \times z\epsilon}{2R}\right) = \frac{Hv}{T(v'_g - v'_l)} \qquad (13)$$

Again assuming that v'_l is negligible compared to v_g at low pressures and the ideal gas law holds, one can write with rearrangement:

$$RT + \frac{N_A \times z\epsilon}{2} = H_v = E_v + P\Delta V \qquad (14)$$

where E_v equals the internal heat of vaporization. If we assume the ideal gas law holds, equation (14) becomes:

$$E_v = \frac{N_A \times z\epsilon}{2} \qquad (15)$$

DERIVATIONS OF THE CORRELATIONS UTILIZED

Liquid Density as a Function of Vapor Pressure

The following is Kemme's derivation based upon Kurata and Isida's equation (11) and presents his relationship between liquid density, vapor pressure and the number of carbon atoms in a straight chain molecule.

Liquid volume is equal to the sum of the volume of full cells plus holes. At low temperatures, i.e. below the normal boiling point, one may assume that the number of empty cells in a liquid is negligible compared to the number of full cells. Therefore, one can say that the liquid volume per molecule, v_l is equal to $x\tau$, the volume of a molecule. The molal liquid density, ρ_l, may then be described as:

$$\rho_l = \left({}^{1}/_{N_A} \quad v_l \right) \tag{16}$$

where N_A is Avogadro's number. Substituting (16) into (11) and noting that $R = N_A k$ yields:

$$\ln P = \ln (RT\rho_l) + x - 1 - \left[\frac{N_A \varepsilon x \gamma}{2TR} \right] \tag{17}$$

Equation (17) may be rewritten into a more useful form as follows:

$$\ln (T f_l) = \left[\ln \left(\frac{P}{R} \right) + 1 \right] + \left[\frac{N_A \varepsilon \psi}{2RT} - 1 \right] x \qquad (18)$$

Consider equation (18) at constant pressure. It can be seen that the term $\left[\ln\left(\frac{P}{R}\right) + 1\right]$ would be a constant and for simplicity the term $\left[\frac{N_A \varepsilon \psi}{2RT} - 1\right]$ is also considered constant. The resultant equation shows $\ln (T f_l)$ linear in x. Thus a plot of $\ln (T f_l)$ vs x should produce a straight line for each pressure considered. By definition, x is a function of the effective chain length of a molecule, which in turn is related to the number of carbon atoms in a chain. It has been shown (5) that the function is well represented by:

$$x = N^{2/3} \qquad (19)$$

where N equals the number of carbon atoms in a chain. Therefore, a plot of $\ln (T f_l)$ vs $N^{2/3}$ should also produce linear isobars. Kemme (5) has shown this is actually the case for the n-alkanes. Therefore one may write:

$$\ln (T f_l) = A + B x \qquad (20)$$

where

$$A = \left[\ln \left(\frac{P}{R} \right) + 1 \right] \qquad (21)$$

and

$$B = \left[\frac{N_A \varepsilon \psi}{2RT} - 1 \right] \qquad (22)$$

Equation (21) shows that A is some linear function of ln P. By setting x in equation (20) equal to zero, one may solve for A at different pressures. Again Kemme has shown that a plot of A vs ln P demonstrates the expected function for the n-alkanes. Similarly B is a function of ln P. Substituting these linear functions for A and B in terms of ln P into equation (18) one obtains:

$$\ln (T \rho_x) = C + D \ln P + E x + F x \ln P \qquad (21)$$

This equation relates the liquid density of any compound in a straight chain homologous series with the effective chain length of the compound and its vapor pressure at a corresponding temperature.

A Modified Kurata-Isida Heat of Vaporization Equation

The following development represents Kemme's derivation of a modified Kurata-Isida Heat of Vaporization correlation.

Equation (13) was given as

$$E_V = \frac{N_A \varepsilon \in}{2} \quad x \qquad (13)$$

Plot of E_V as a function of x should be linear, since all the terms except x on the right hand side of equation (13) are constants. A plot of E_V as a function of x, where x equals $N^{2/3}$ shows a linear relation between E_V and x; however contrary to equation (13), this relation is also a function of vapor pressure. Kemme (5) has shown

this to be true for n-alkanes, noting a common intercept at x = 0 and $E_V = 0$. Figures 1, 2, 3, 4, 5, 6, 7 and 8 all show the same linearity but different intercepts for the series which were investigated in this study. Kemme has shown that a plot of the slopes of these curves as a function of pressure displays linearity in ln P.

Therefore at constant pressure one may write:

$$E_V = A + B\,x$$

where

$$B = \frac{N_A \, z \, \epsilon}{2} \qquad (23)$$

and A is a constant characteristic of the series in question.

From the foregoing discussion one is justified in writing:

$$B = C + D \ln P \qquad (24)$$

Combining equations (23) and (24) one obtains an equation which describes the relationship of internal energy of vaporization as a function of vapor pressure and effective chain length for a homologous series of organic liquids. Therefore:

$$E_V = A + C\,x + Dx \ln P \qquad (25)$$

Figure 1
ALCOHOLS

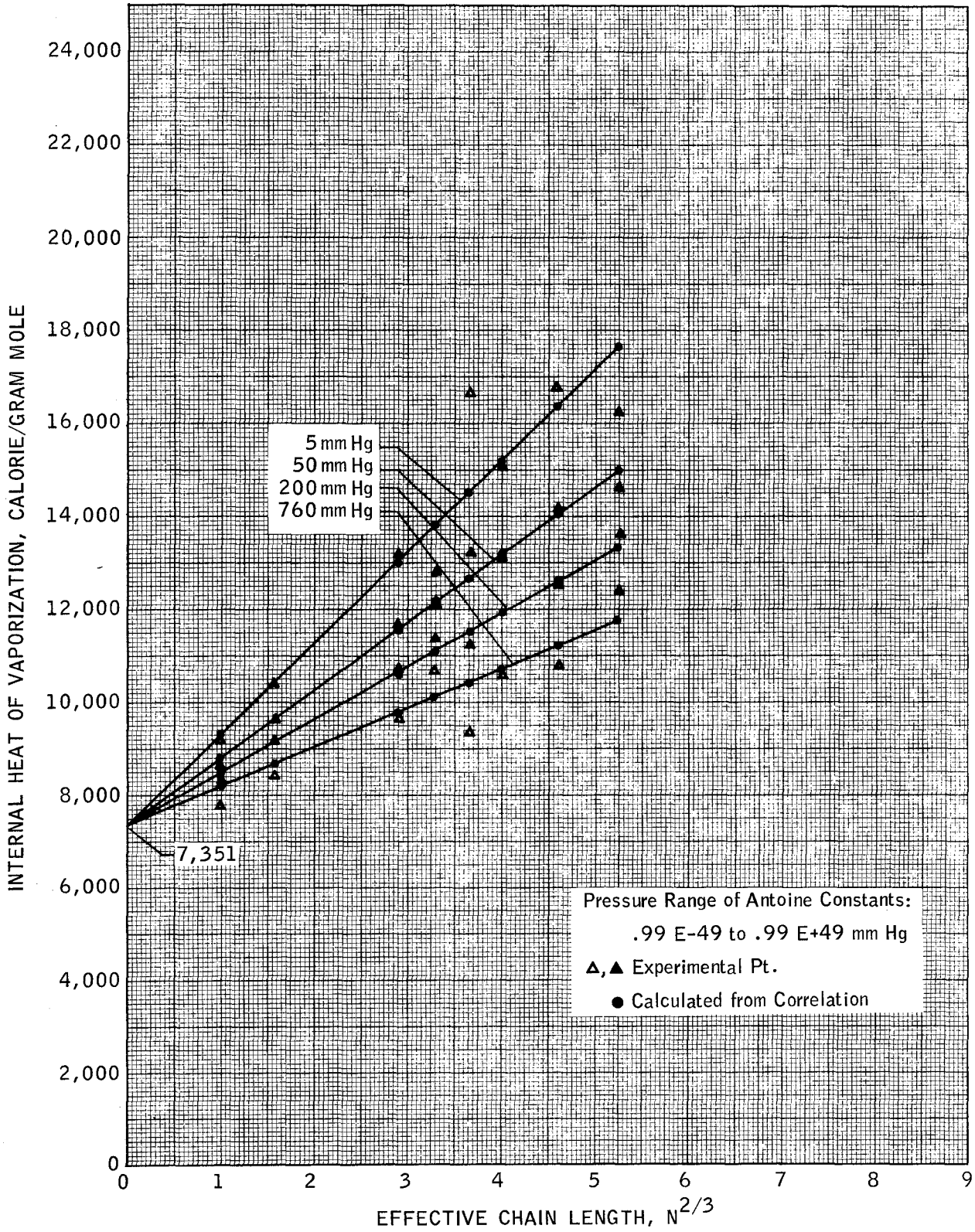


Figure 2

ALCOHOLS

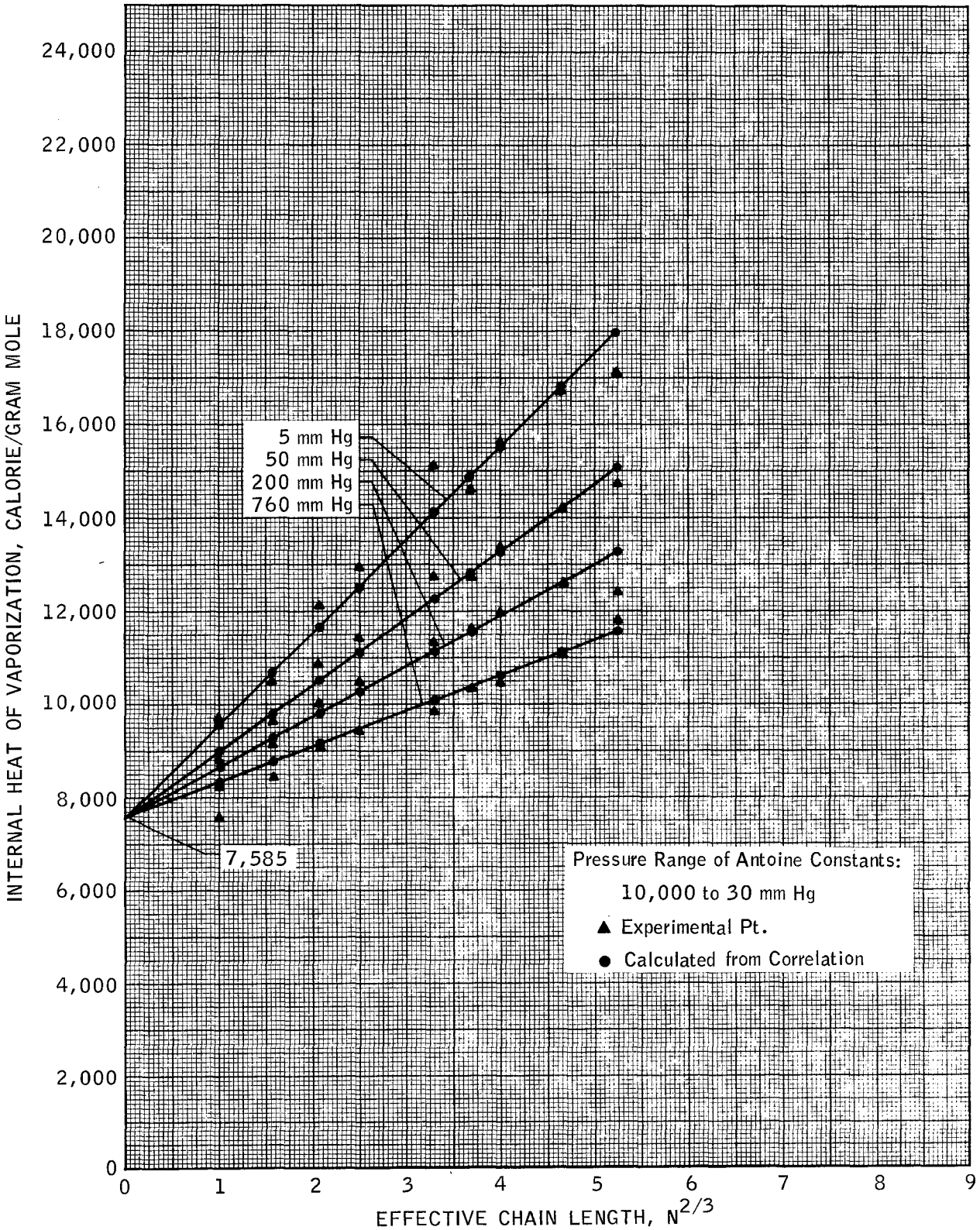


Figure 3

n-AKYL CHLORIDES

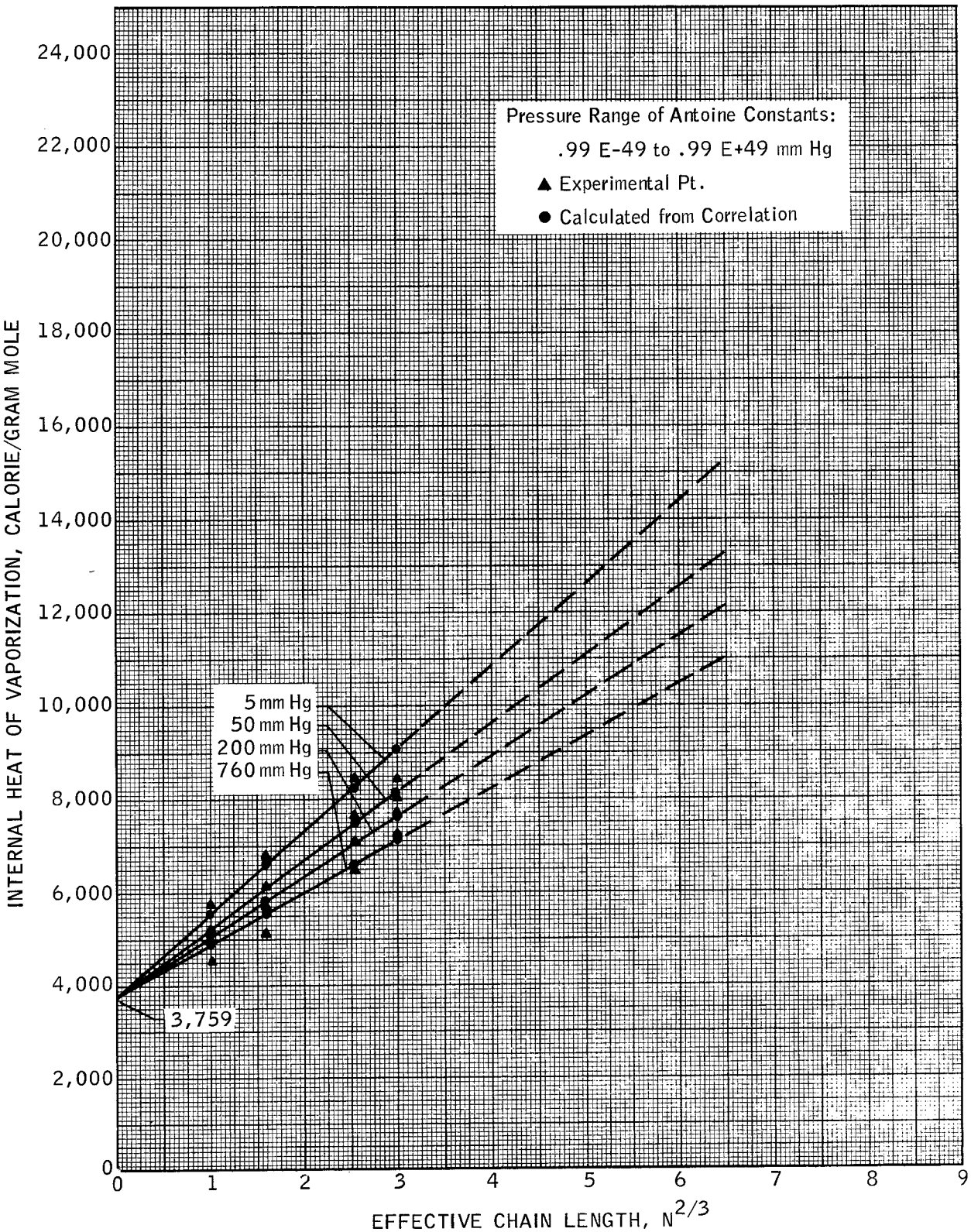


Figure 4

n-ALKANOIC ACIDS

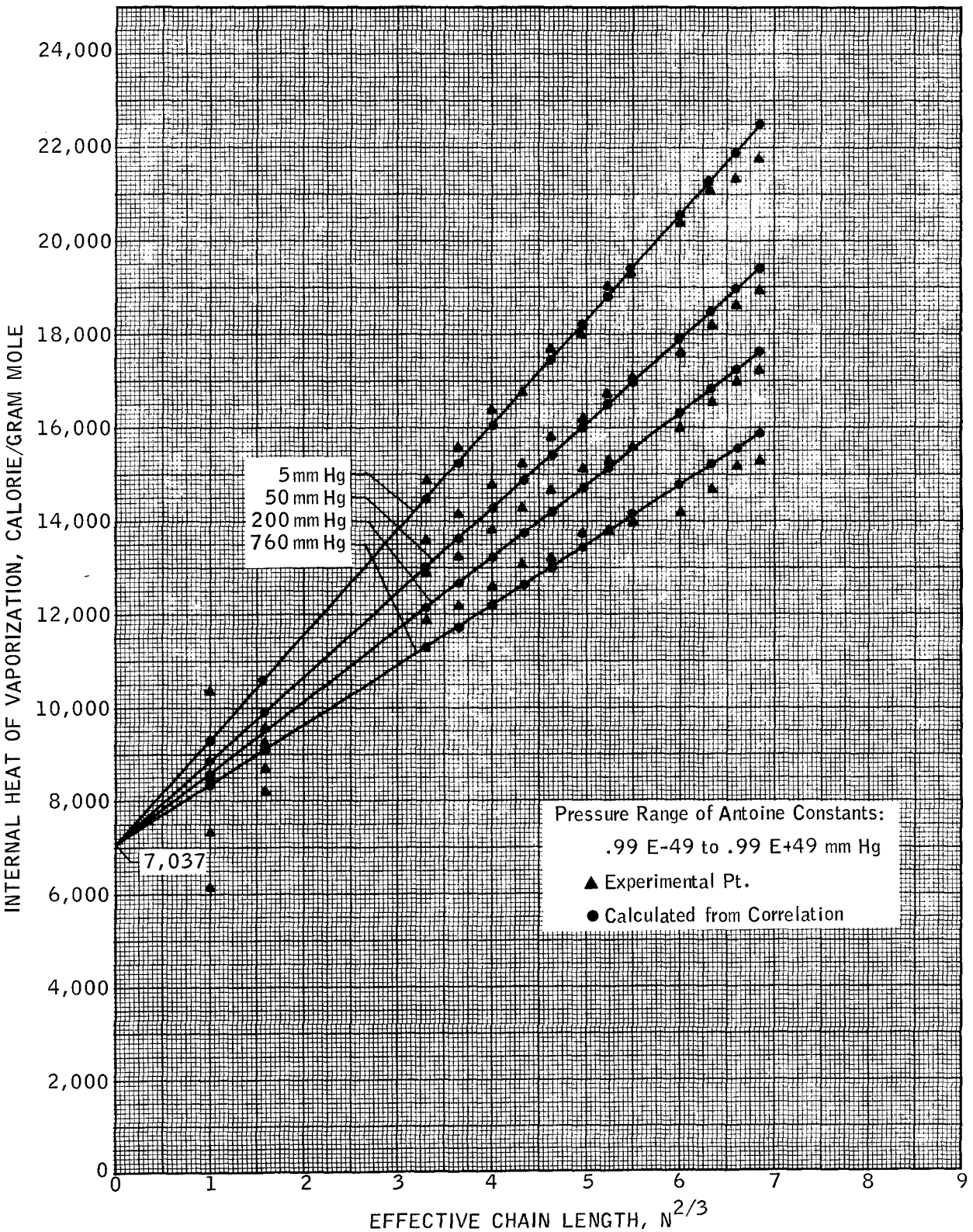


Figure 5

n-ALKANOIC ACIDS

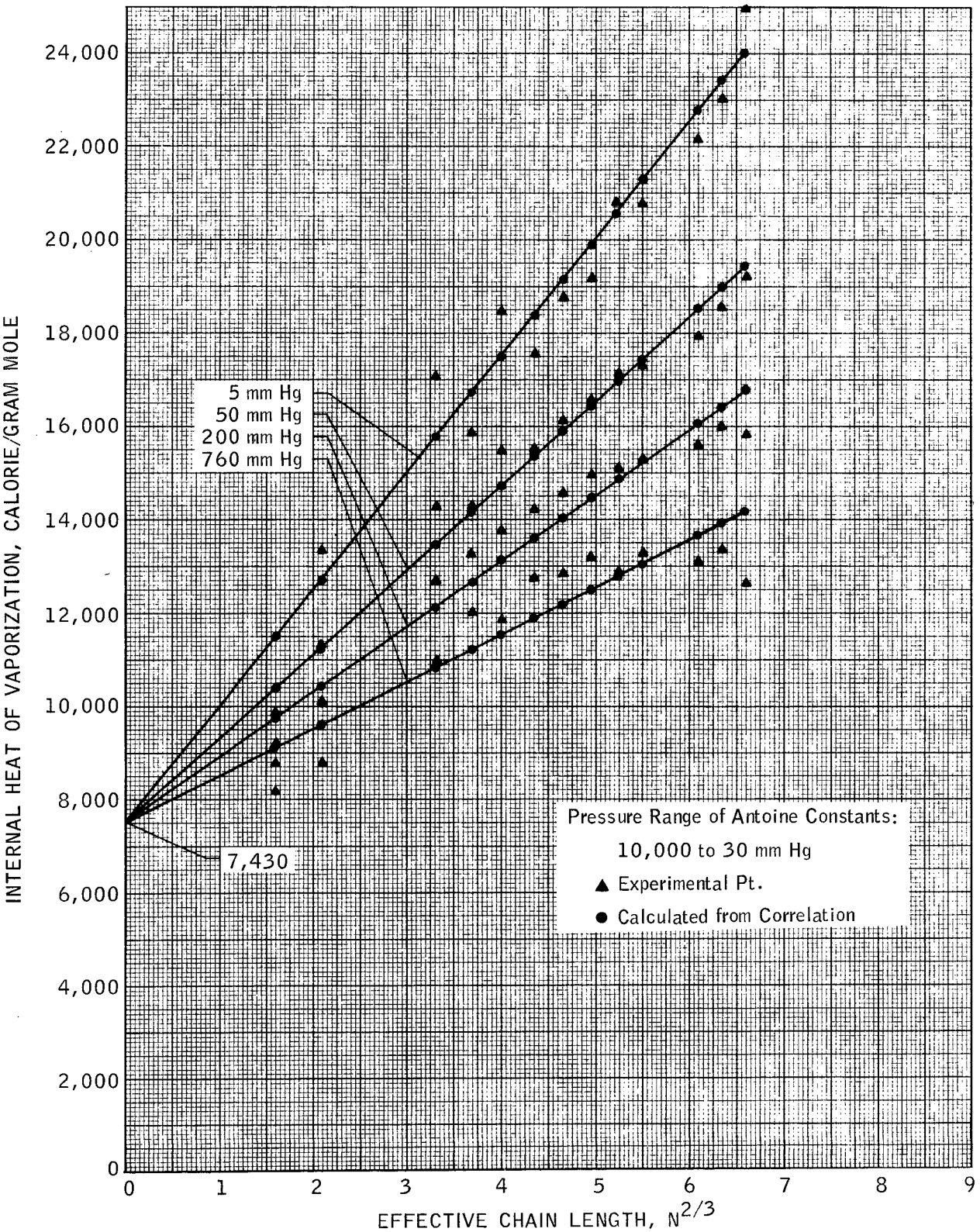


Figure 6

ESTERS - FORMATE

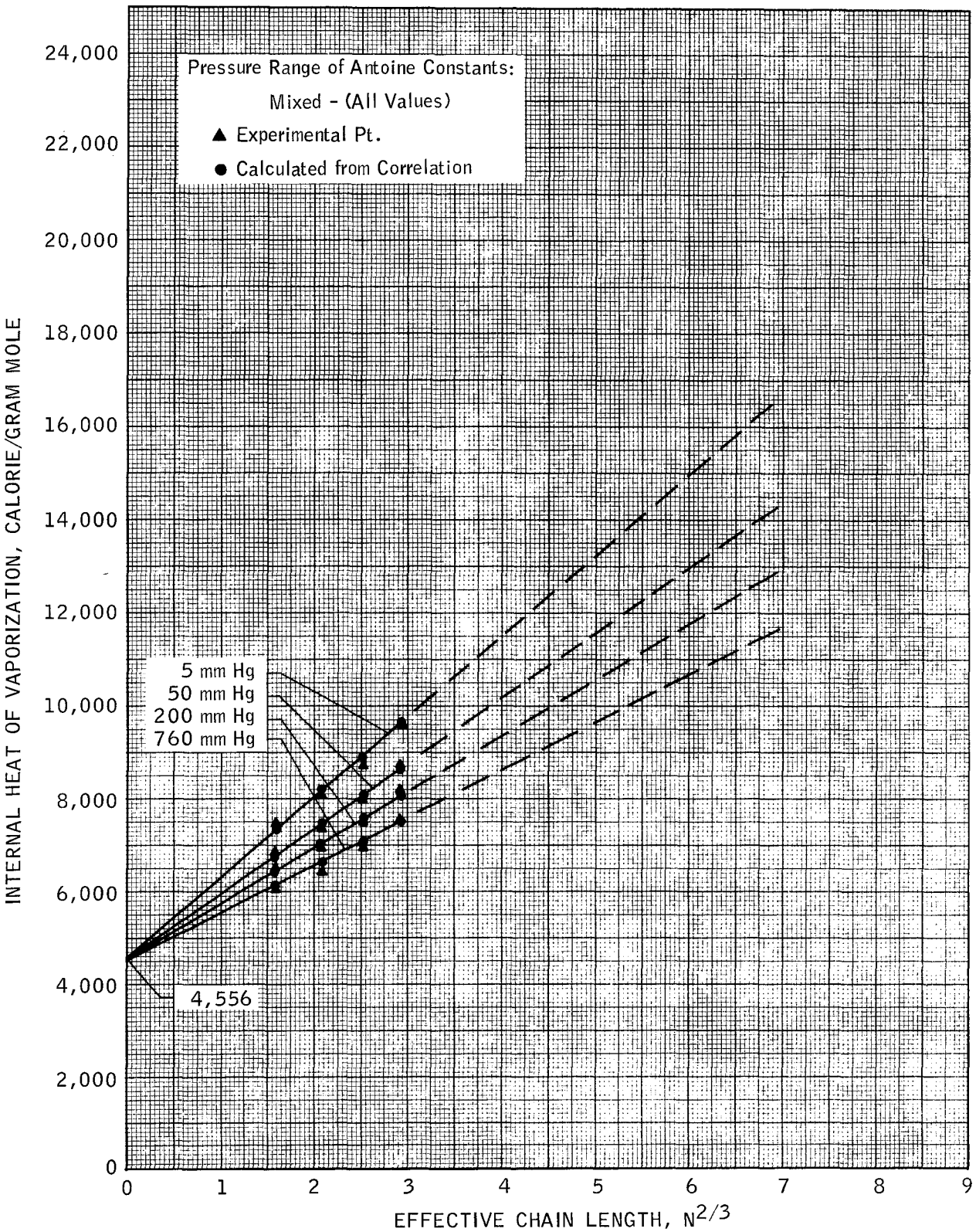


Figure 7

n - AKYL BENZENES

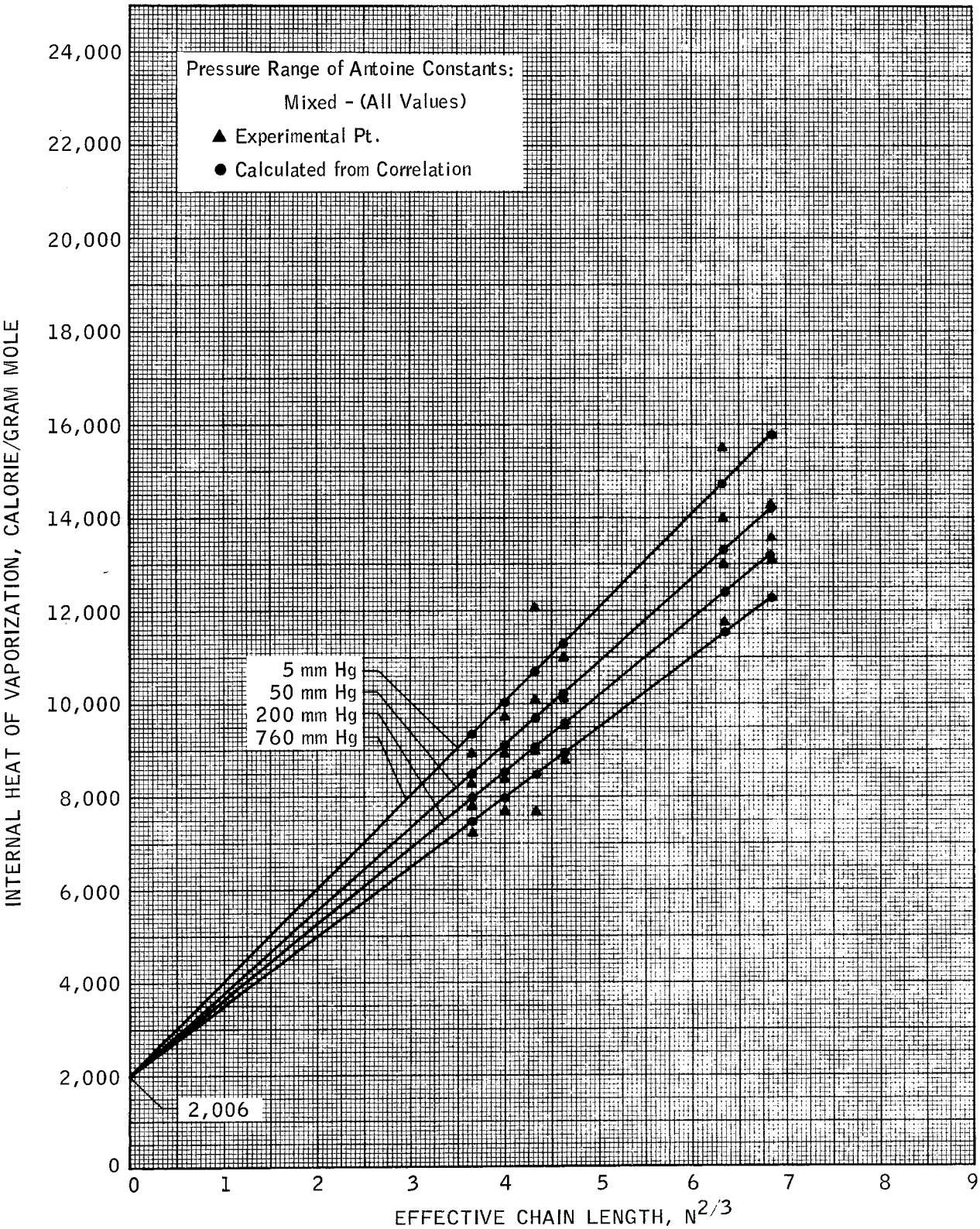
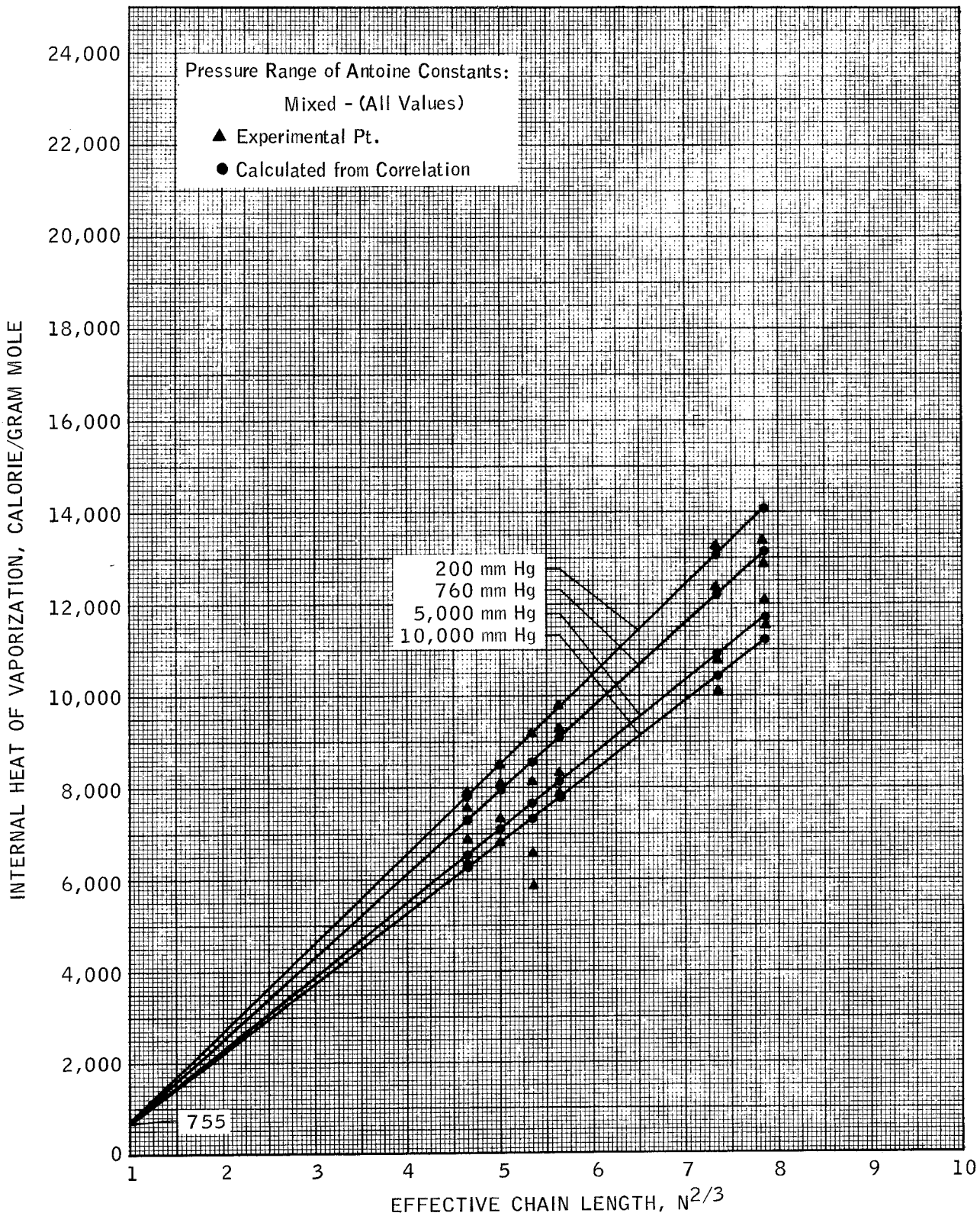


Figure 8

n - AKYL BENZENES



APPLICATION OF CORRELATIONS AND RESULTS

The Density Correlation

The derived density correlation was presented as:

$$\ln (T \rho_l) = C + D \ln P + Ex + Fx \ln P \qquad (26)$$

The validity of this equation may be tested by evaluating the constants and comparing the calculated density values with experimental values. These constants were evaluated using the method of least squares multiple linear regression analysis (9). The following substitutions were made in order to linearize the equation:

$$\ln (T \rho_l) = y$$

$$\ln P = x_1$$

$$x \ln P = x_2$$

this results in

$$y = C + Dx_1 + Ex + Fx_2 \qquad (27)$$

The computational analysis of this equation was performed on an IBM-360/65 system. A complete listing of this program as used along with instructions for input sequence and nomenclature may be found in the Appendix.

As can be readily seen from the program listing, temperature-density data points for the homologous series were read into storage with the Antoine constants for each compound. From these the vapor pressure could be generated at any point. The least squares analysis was performed on these data, the constants established and a statistical analysis of the correlation, yielding such information as the correlation coefficient, the sum of the squares of regression, the residual sum of the squares and the variance of the estimate, was generated Using the established coefficients the program then calculated the densities at each of the input temperatures, and made a point by point comparison of the calculated versus the experimental data. This comparison yields a percent error for each point along with an overall average and absolute maximum percent error for the data set.

Heat of Vaporization Correlation

The modified Kurata-Isida heat of vaporization equation was presented in equation (25) as:

$$E_V = A + Cx + Dx \ln P \qquad (25)$$

Again, the constants in this equation were evaluated using the method of multi-linear regression analysis. The following substitutions were utilized to linearize the equation:

$$E_V = y$$

$$x_1 = x\ln P$$

yielding

$$y = A + Cx + Dx_1 \tag{28}$$

The multi-linear regression analysis of this equation was effected according to Volk (10). Computational work was performed on an IBM 360/65 system. The program was originally designed so that only the Antoine constants for each compound in the series to be analysed had to be supplied. From this information the program generates the heat of vaporization data. A complete listing of this program as used along with instructions for input sequence and the nomenclature may be found in the Appendix.

This program yielded a statistical analysis of the correlated data set, as well as a point by point comparison of calculated versus experimental value.

Variation of Effective Chain Length Parameter

In order to determine the optimum power of the effective chain length parameter, x (up to this point assumed to be two-thirds) Kemme set up the following generalized function:

$$x = N^y \tag{29}$$

where N equals the number of carbon atoms in the chain. In order to establish the optimum y the correlation was carried out with different powers of N. The variance of the estimate of the least squares line for each power was plotted against the power. The power which produced the minimum variance of the estimate was chosen as the optimum.

This method was applied to all the series considered in this thesis. The results of these plots may be seen in Figures 9, 10, 11, 12, 13, 14, 15, 16, 17 and 18.

Figure 9

MULTILINEAR REGRESSION OF INTERNAL HEAT OF VAPORIZATION CORRELATION ALCOHOLS

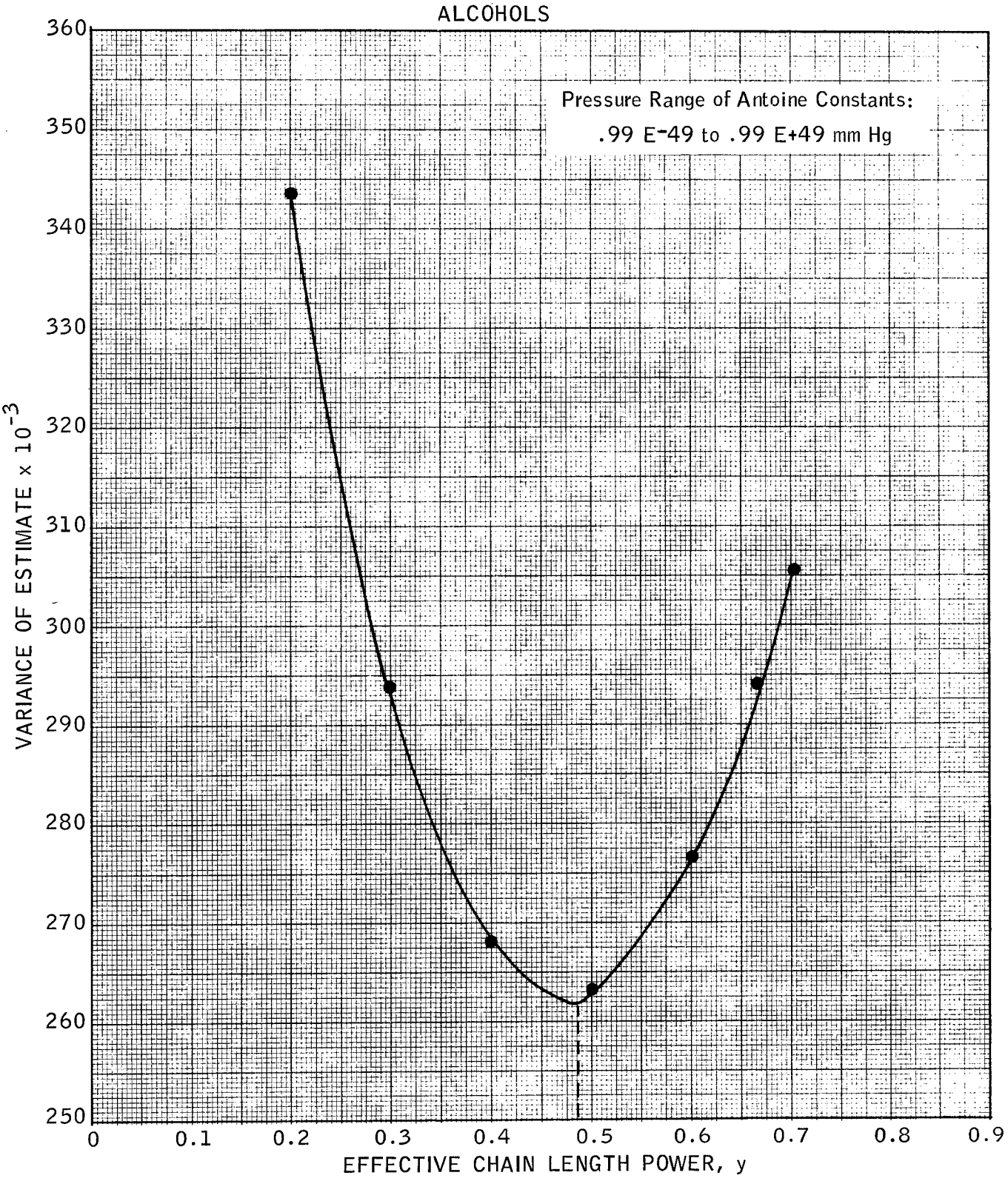


Figure 10

MULTILINEAR REGRESSION OF INTERNAL HEAT OF VAPORIZATION CORRELATION ALCOHOLS

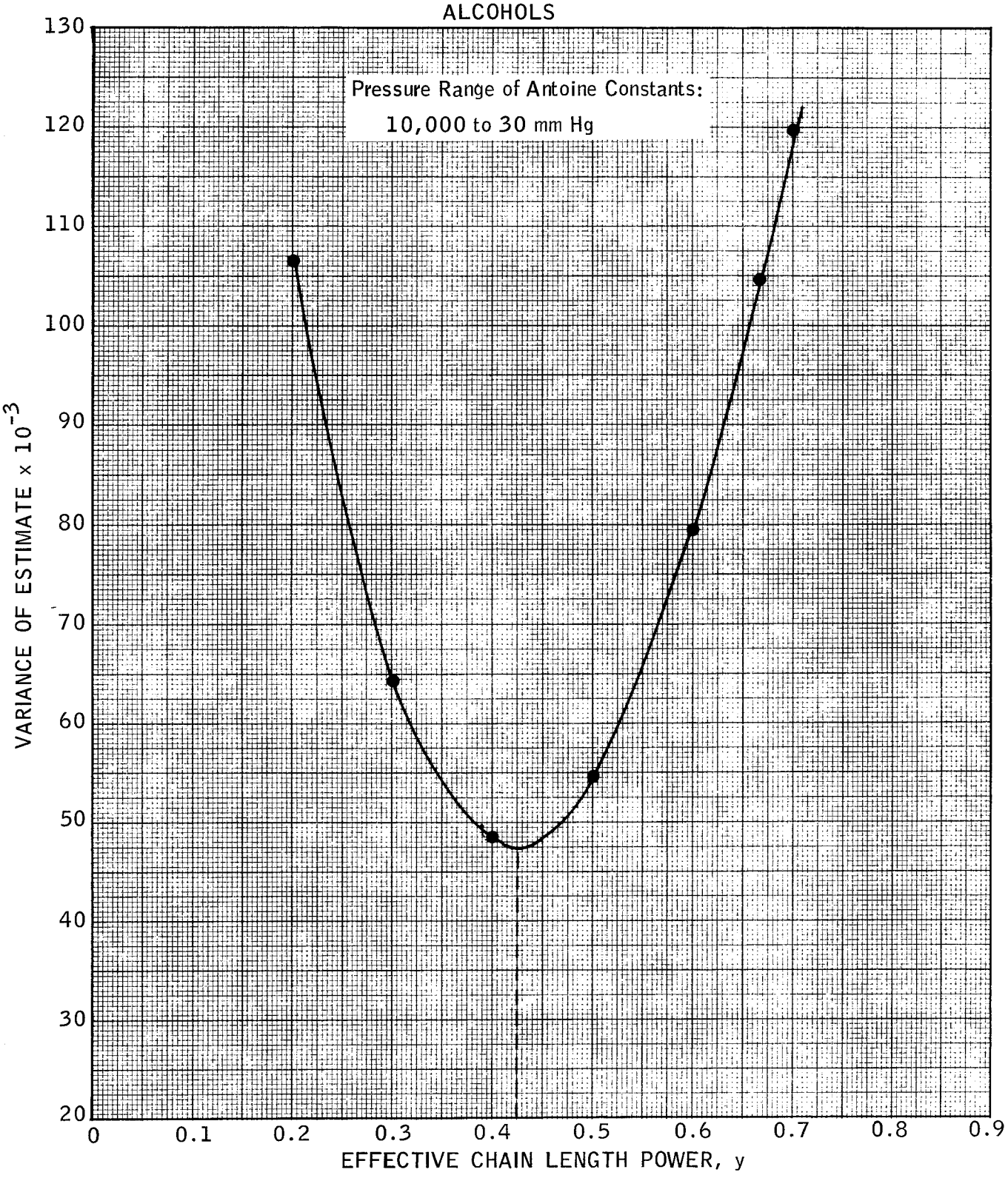


Figure 11

MULTILINEAR REGRESSION OF INTERNAL
HEAT OF VAPORIZATION CORRELATION
n-ALKYL CHLORIDES

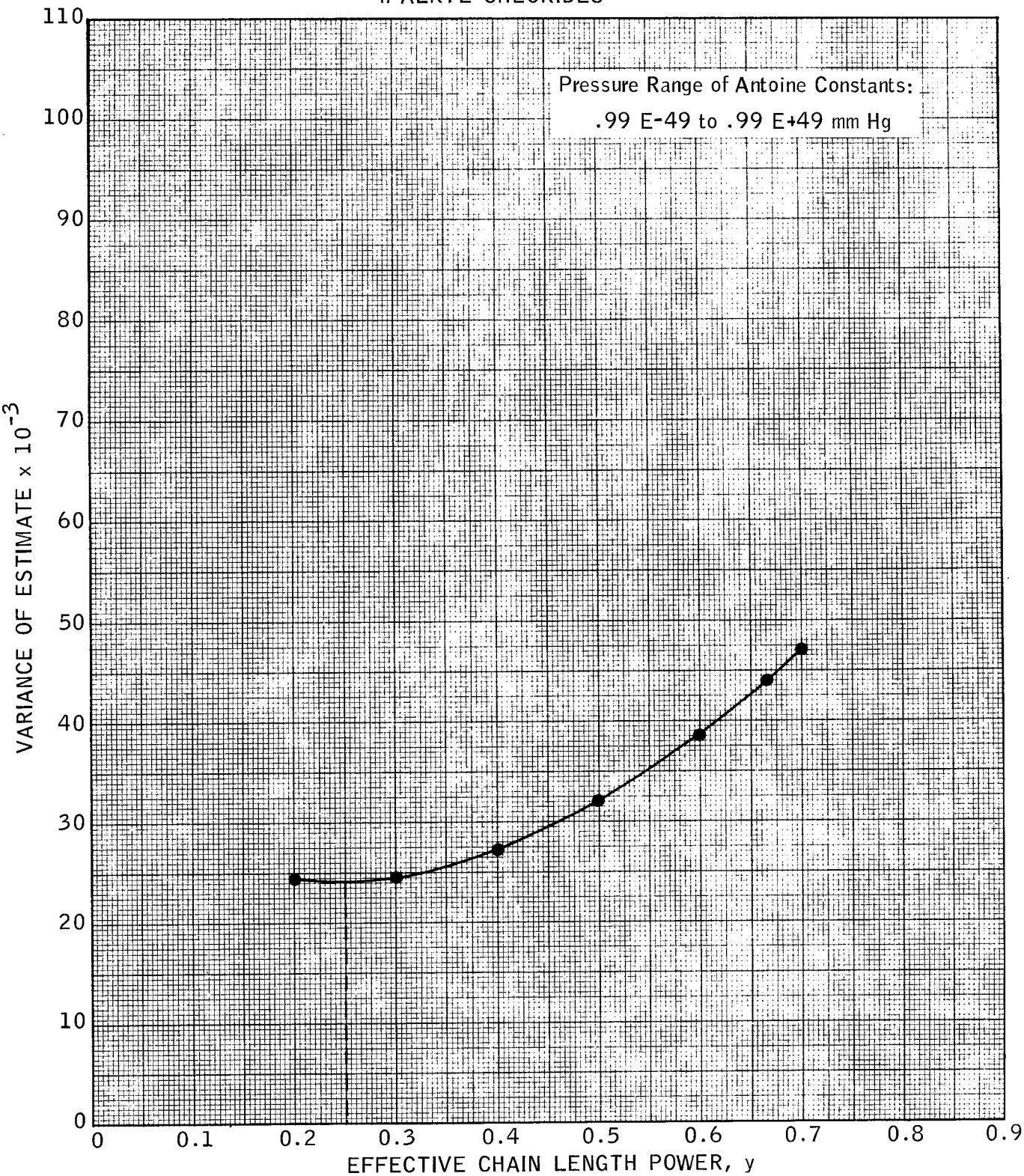


Figure 12

MULTILINEAR REGRESSION OF INTERNAL
HEAT OF VAPORIZATION CORRELATION
n-ALKANOIC ACIDS

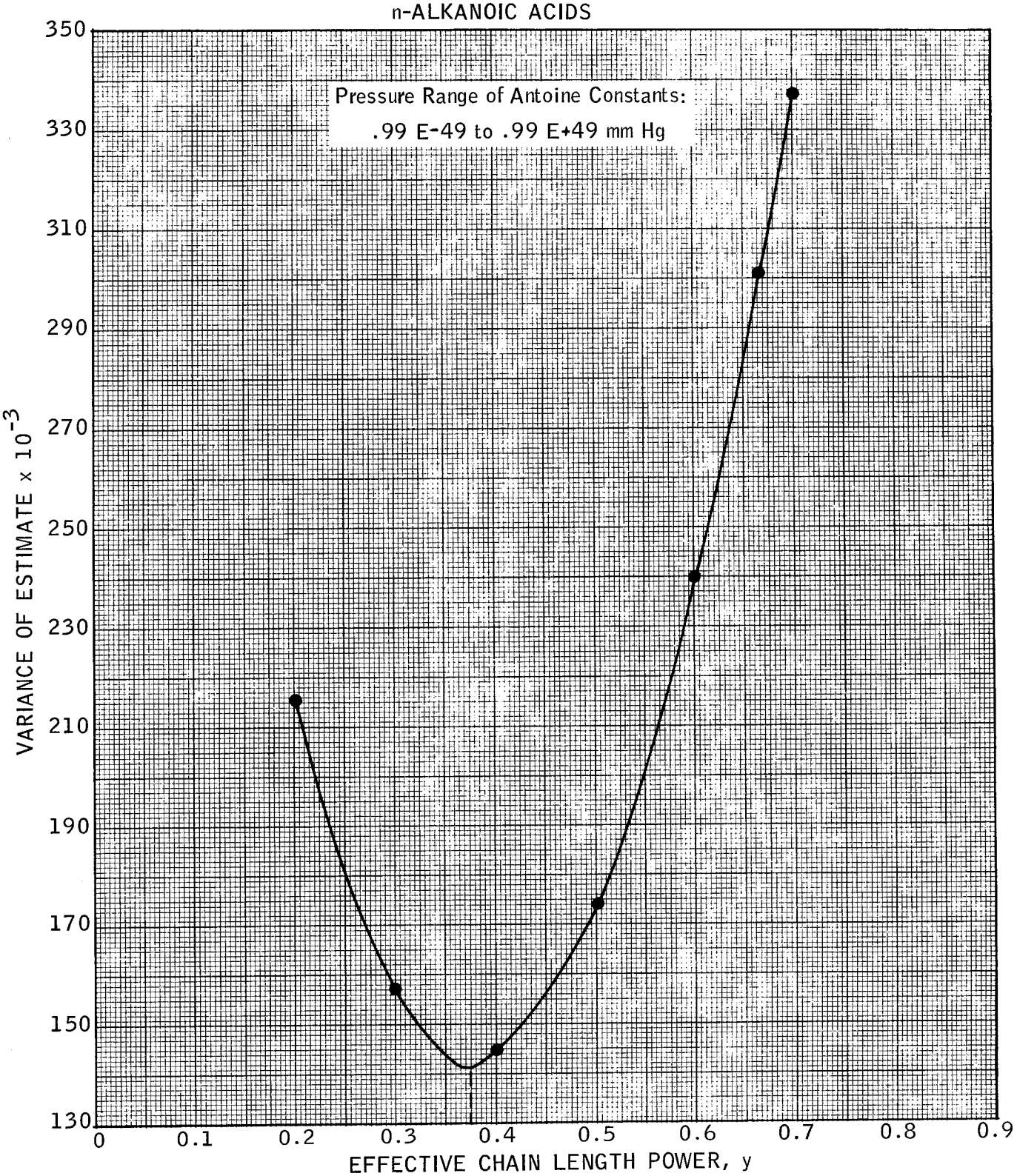


Figure 13

MULTILINEAR REGRESSION OF INTERNAL
HEAT OF VAPORIZATION CORRELATION
n-ALKANOIC ACIDS

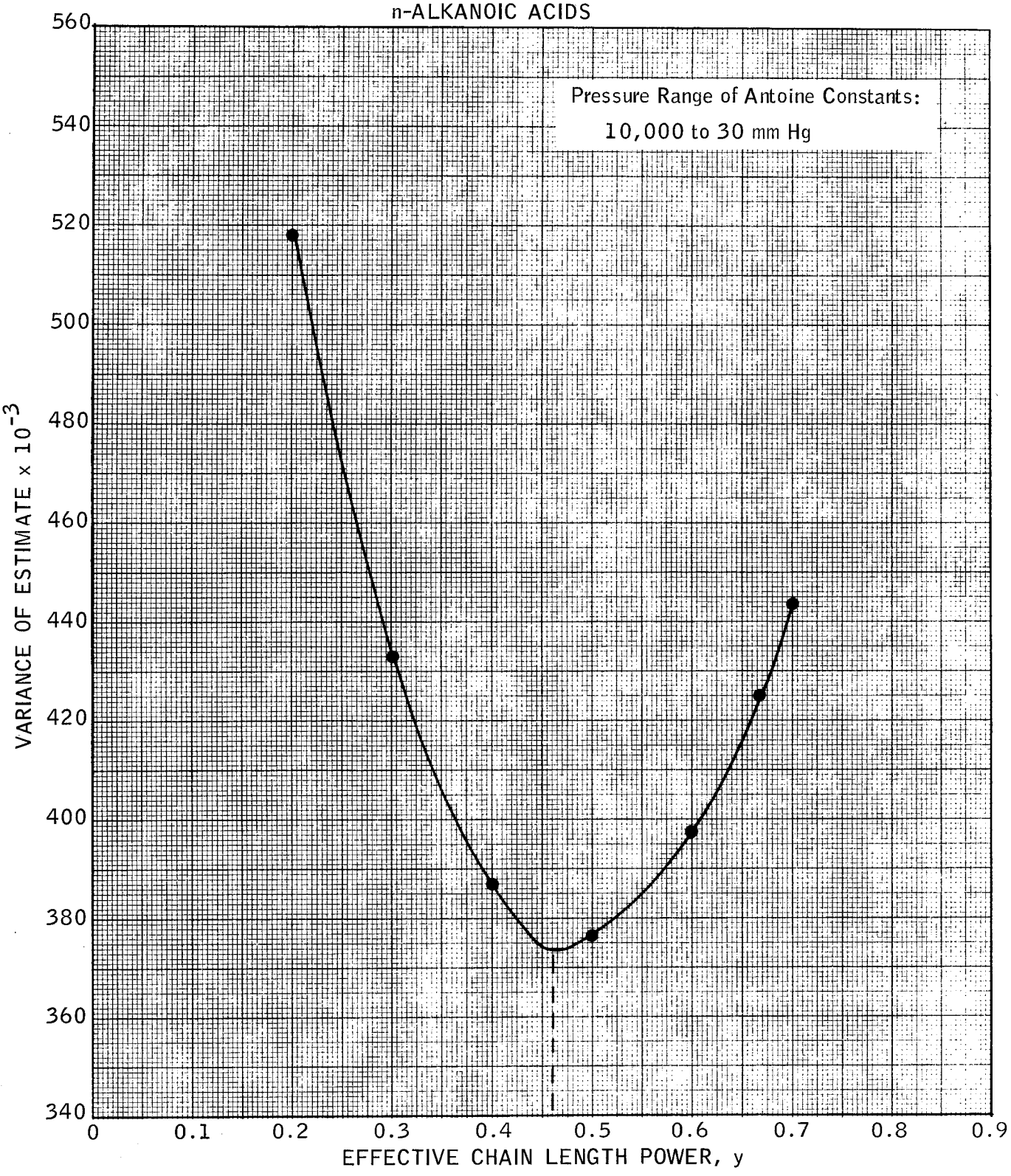


Figure 14

MULTILINEAR REGRESSION OF INTERNAL
HEAT OF VAPORIZATION CORRELATION
ESTERS-FORMATE

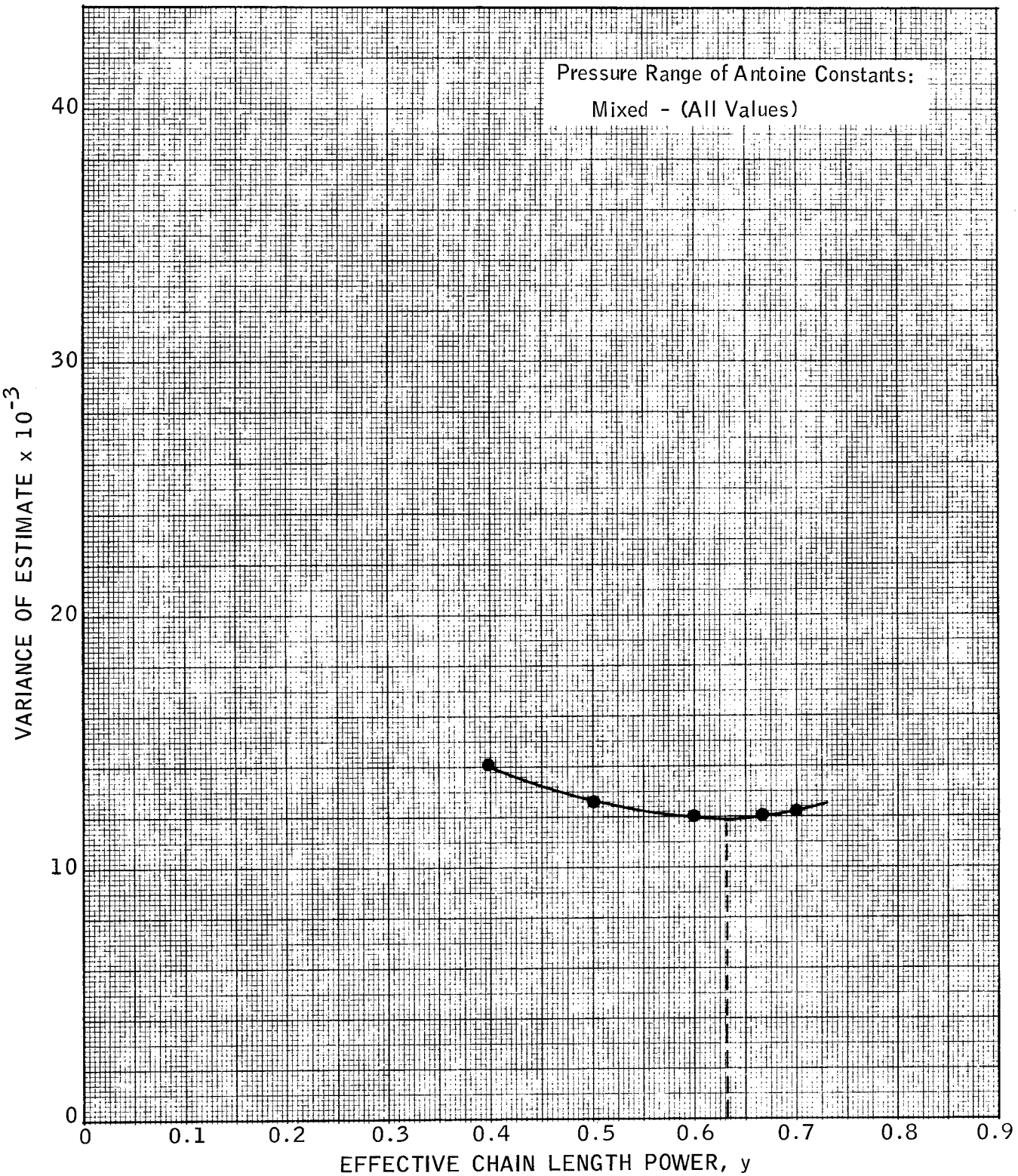


Figure 15

MULTILINEAR REGRESSION OF INTERNAL
HEAT OF VAPORIZATION CORRELATION
n - ALKYL BENZENES

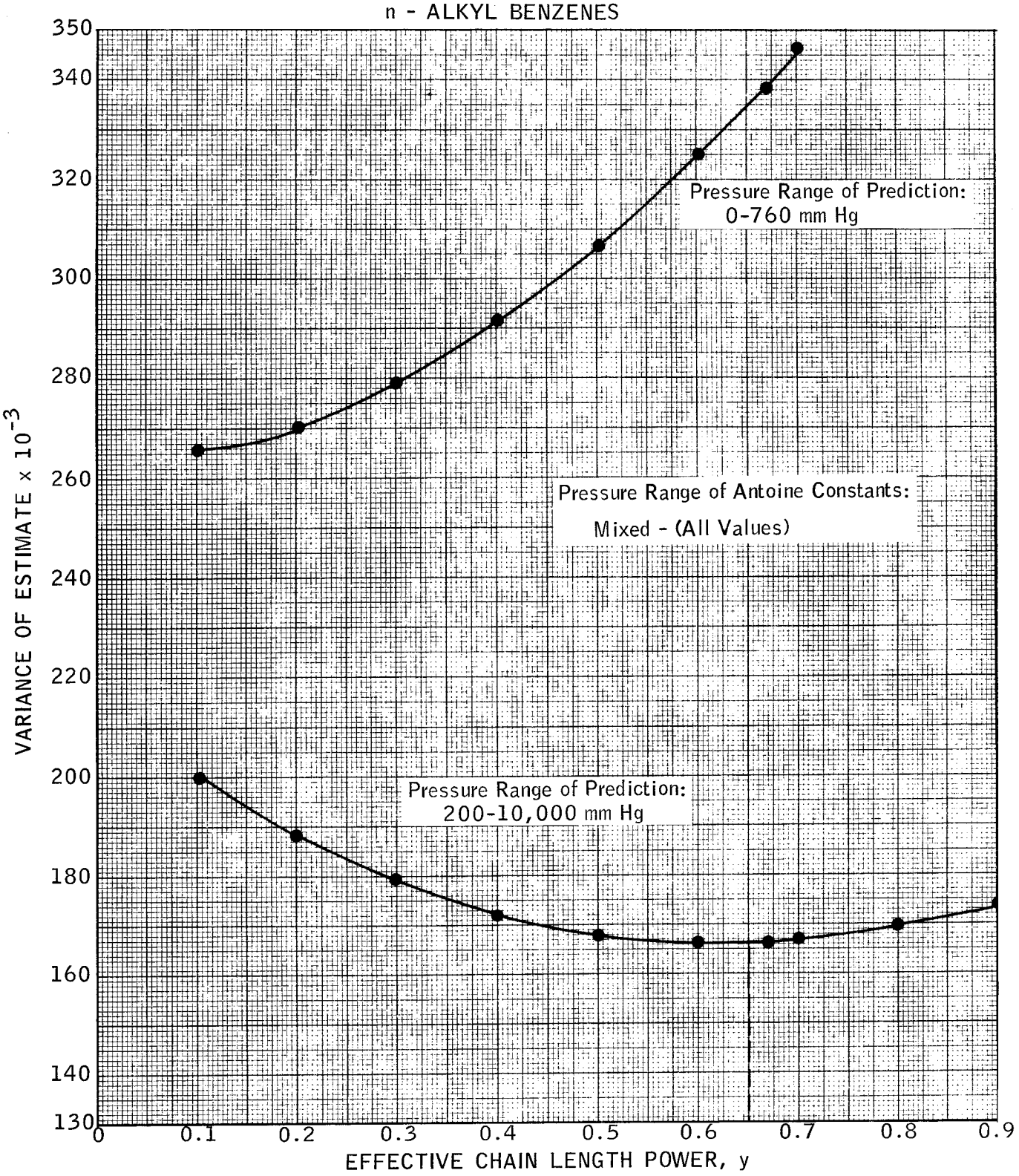


Figure 16

LINEAR REGRESSION OF DENSITY CORRELATION
n-ALKANOIC ACIDS

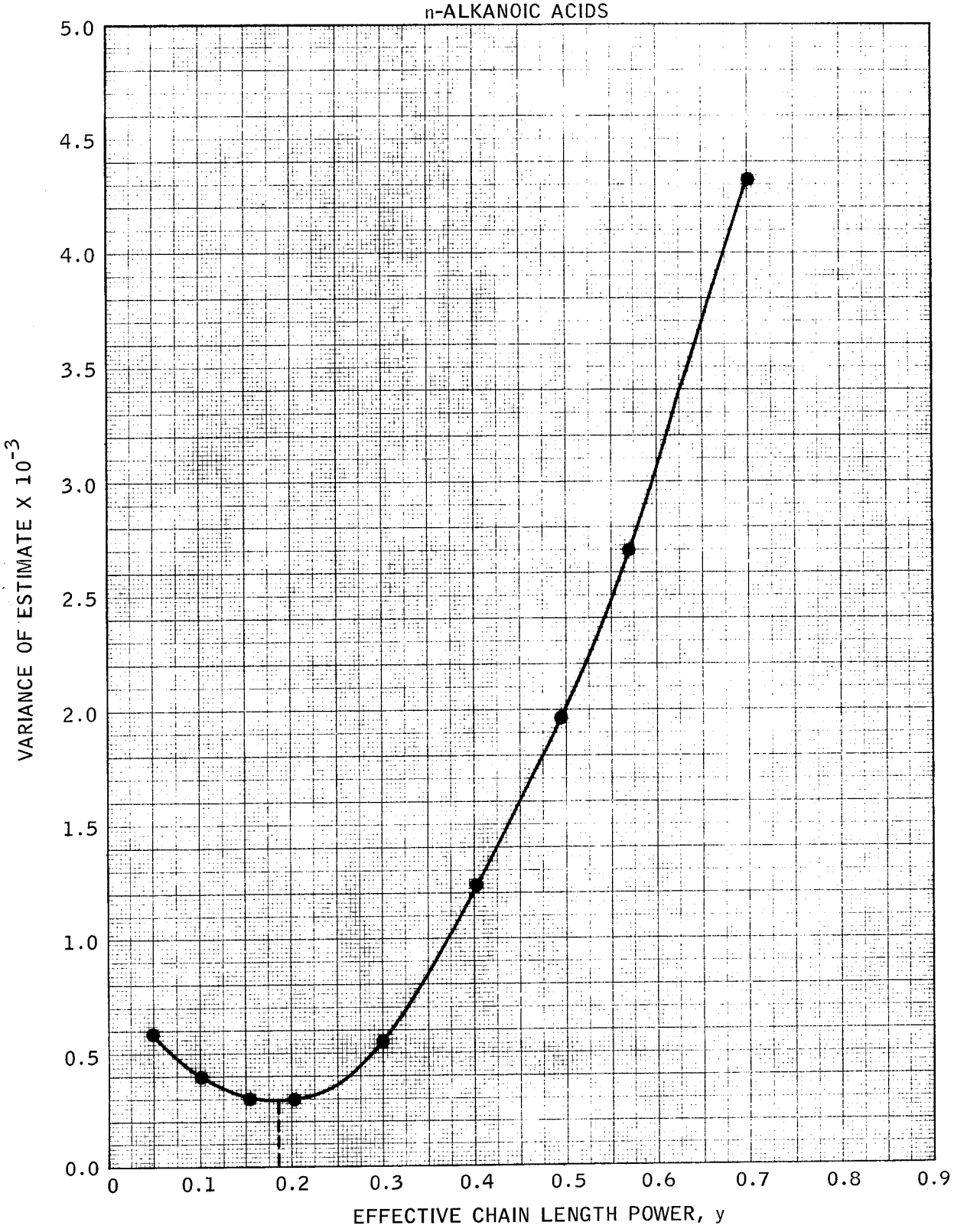


Figure 17

LINEAR REGRESSION OF DENSITY CORRELATION
ESTERS-FORMATE

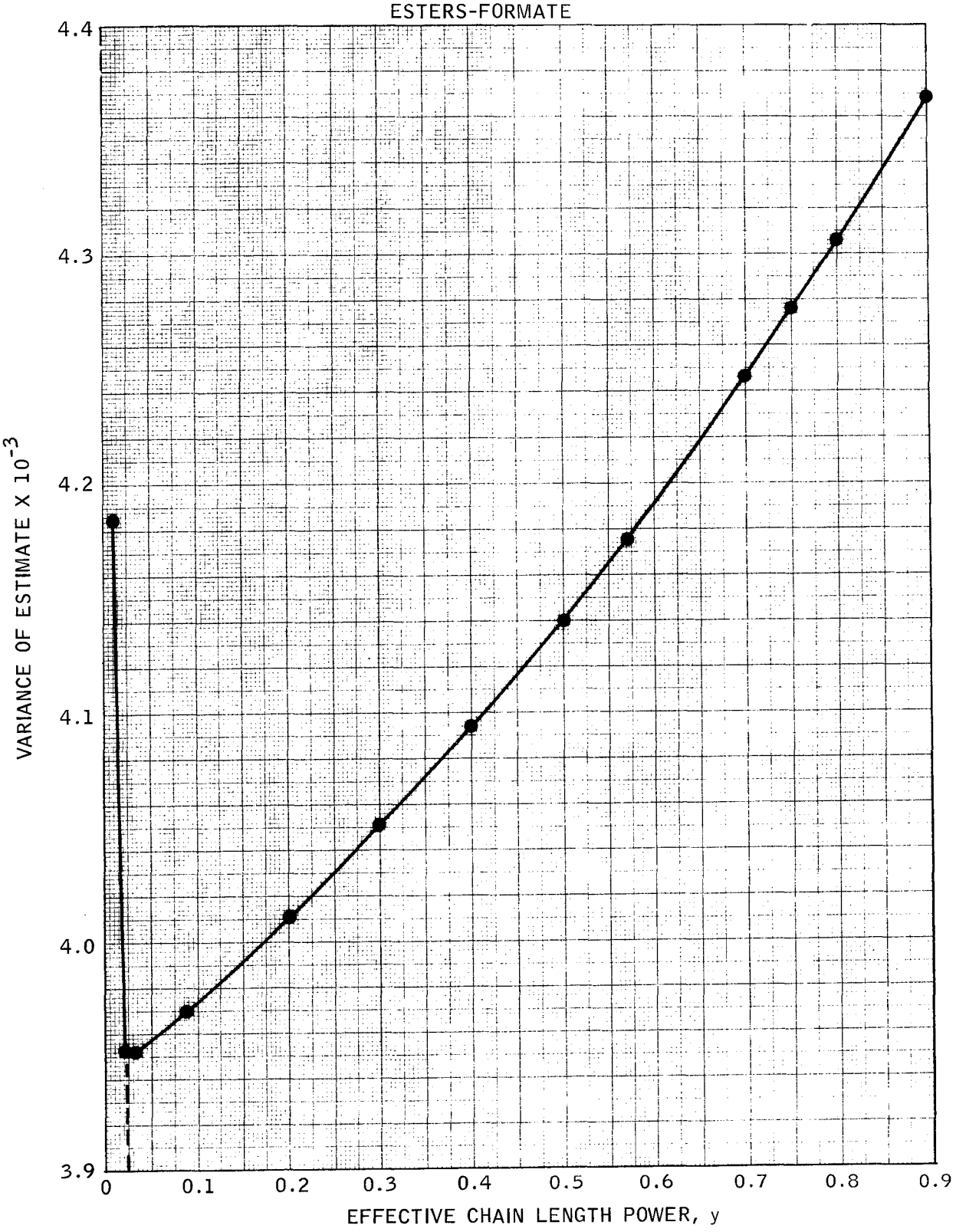
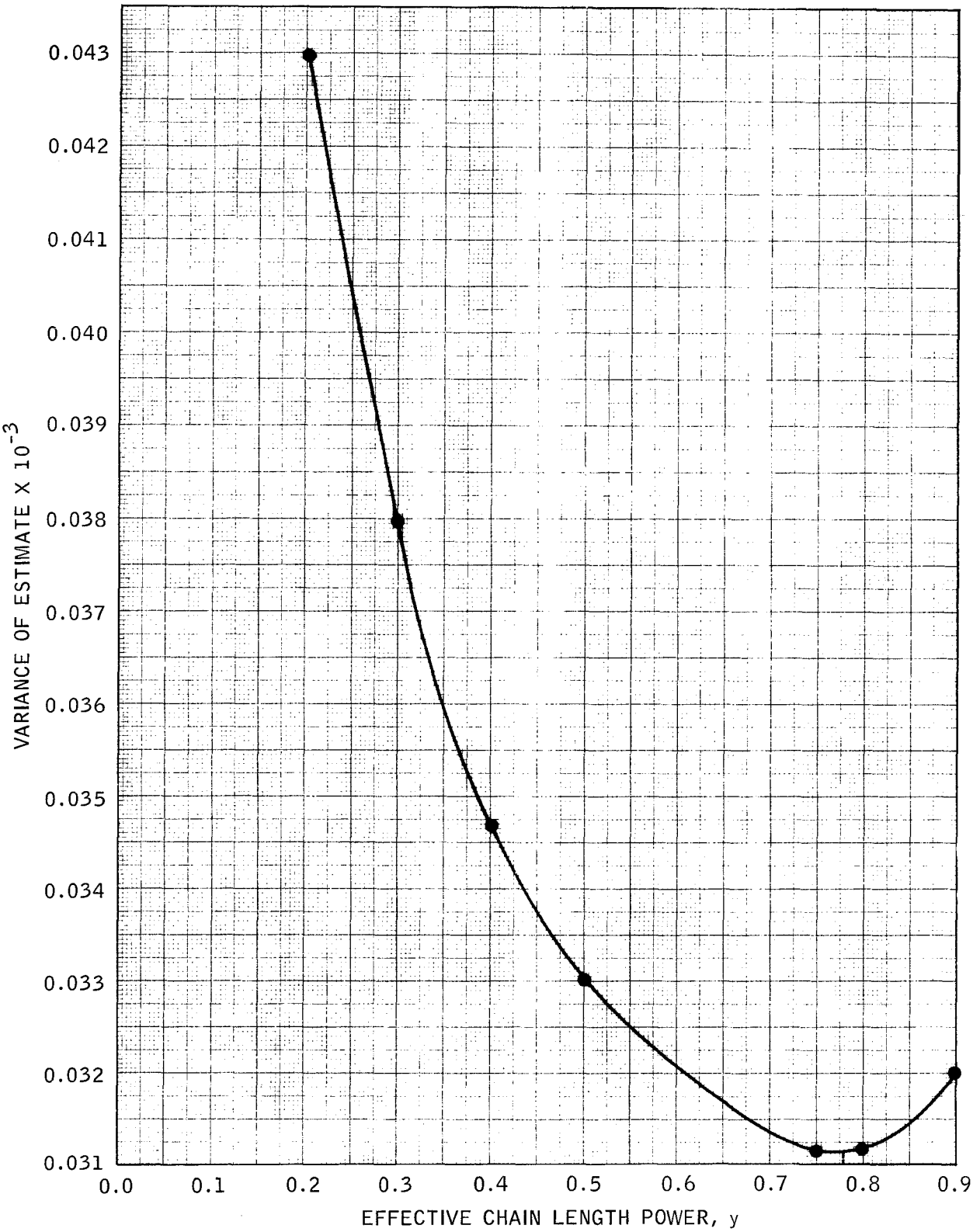


Figure 18

LINEAR REGRESSION OF DENSITY CORRELATION
n - ALKYL BENZENES



Data Sources

Density data for the homologous series investigated are presented in Appendix B. The source reference is indicated for each piece of data. Data is listed for the most recent reference available for a given point, as it was felt that this would be most reliable.

Appendix C presents a complete listing of catalogued Antoine constants for a number of homologous series including those investigated. All Antoine constants used in this work are presented.

Heats of Vaporization Generated From Antoine Constants

The Haggenmacher method (3), and Fishtine's method (2) for calculating the delta compressibility factor, ΔZ, were utilized to calculate the internal heats of vaporization from vapor pressure data, as described by Kemme (5);

The Haggenmacher equation has as its basis the Clapeyron equation in the following form:

$$\frac{d \log P}{d (1/T)} = - \frac{Hv}{2.303R(Zg-Z_1)} \qquad (30)$$

The Antoine equation differentiated with respect to 1/T is:

$$\frac{d \log P}{d (1/T)} = \frac{T^2 B}{(t + C)^2} \qquad (31)$$

Subtracting (31) from (30) results in:

$$H_V = \frac{2.303\ RT^2\ B\ \Delta Z}{(t + C)^2} \tag{32}$$

upon rearrangement. Where ΔZ equals $Z_g - Z_l$.

Since; $$H_V = E_V + P\ \Delta V \tag{33}$$

and, $$\Delta V = \frac{RT}{P}\ \Delta Z \tag{34}$$

by substitution one obtains:

$$E_V = \frac{2.303\ RT^2\ B\ \Delta Z}{(t + C)^2} - RT\ \Delta Z \tag{35}$$

Equation (35) was utilized to generate internal heats of vaporization in the heat of vaporization correlation program.

Results

The modified Kurata-Isida heat of vaporization equation was tested by applying it to the following homologous series: n-alcohols, n-alkyl chlorides, n-acids, formate esters and n-alkyl benzenes.

The results of the multi-linear regression of the Antoine constants for these series, as listed in Appendix C, is given in Appendix D. The optimum power, y, of the carbon number, N, was determined for each series considered by substituting various powers of N in the regression analysis and plotting the resulting variance of the estimated regression line versus the power used, on a linear plot. The result yielded a minimum variance for each series at discreet powers, as shown in Figures 9 through 15. Since it was verified by this work that the correlation is not extremely sensitive to y, as determined by Kemme (5), a value of 0.666 was used for the power, PW, for all the results shown in order to provide a consistent basis of comparison.

The Kemme-Kreps density equation was tested by applying it to the following series: n-acids, formate esters and n-alkyl benzenes.

A summary of the results for the series investigated is presented in Table 1. Plots of the chain length power versus the variance of the estimate are given in Figures 16, 17, and 18. The entire set of data presented in Appendix B was utilized in the determination of these results.

Series Name	n-Acids	n-Esters Formate	n-Alkyl Benzenes
No. of Density Data Points	51	36	31
Optimum y	0.19	0.03	0.78
C constant	4.3000	31.5087	1.6075
D constant	0.0801	- 1.5883	0.0820
E constant	- 2.3833	- 29.2698	- 0.1599
F constant	- 0.0419	1.5506	- 0.0081
Sum of Squares of Regression	22.712	0.942	0.840
Correlation Coefficient	0.9997	0.9372	0.9995
Variance of Est. of ln (TPx)	2.96×10^{-4}	39.53×10^{-4}	0.3173×10^{-4}
Avg. Absolute Error, %	1.308	4.535	0.359
Max. Absolute Error, %	5.927	22.829	2.213

Table 1 Results of Density Correlation

Discussion of Results

Density Correlation

The effective chain length, x, has been defined as a function of the number of carbon atoms in a chain raised to some power, y; the method for determining the optimum y for any given homologous series has been discussed previously. For the series under consideration here, the following are the optimum values of y:

n-acids	0.19
formate esters	0.03
n-alkyl benzenes	0.78

as determined by regression of the data sets presented in Appendix B.

Kemme (5) has shown that the correlation is not very sensitive to y, in the vicinity of the optimum y for a given series. Kemme (5) reported the following optimum values of y for the homologous series he considered:

n-alkanes	0.57
n-alkenes	0.68
n-alkyl chlorides	0.55
n-alcohols	0.20

Kemme has suggested that the reason the effective chain length is a function of the number of carbon atoms raised to a

power rather than being a direct linear function of this parameter is the disparity in the cell size of the end group involved in the homologous series under investigation versus the cell size of the center segment of the chain e.g. a $-CH_2-$ segment. Thus, if all carbon groups in the chain occupied equal volumes, a linear function might be in order. Since the end groups are larger than the center segments this is clearly not the case. Further, as the length of the chain increases, the effect of the spacially larger end group diminishes; and, in addition, increasing the length of the chain introduces a greater number of degrees of freedom, thus allowing the molecule to assume a lesser volume. Since these effects manifest themselves during the addition of the first carbon atoms in the chain, the addition of further carbon atoms results in a more linear increase in the effective length. Kemme has concluded that the effective chain length is best described as a power of N. The work of this thesis seems to bear this out.

Kemme has further suggested that different terminal groups on a molecular chain do not seem to influence the effective chain length parameter, y. This conclusion is based upon his reported optimum values of y for the n-alkanes, n-alkenes and n-alkyl chlorides which are grouped about the 0.6 point; the value he suggests may be taken as that for these series without introducing significant error. He points out however that the value he reports for the n-alcohols of 0.20 seems to be a glaring exception to the

rule. This might be explained by the existence of hydrogen bonding present in the alcohols, resulting in a greater attraction between molecules and thus a more compact molecular structure, were it not for the fact that Kemme finds the optimum effective chain length parameter for the homologous series he considers in the heat of vaporization correlation to be of the same order e.g. 0.68. The results of this thesis however would seem to substantiate his hypothesis in that the optimum value of y reported for the n-acids, of 0.19, would seem to group this series with the n-alcohols in the same manner as Kemme groups the n-alkanes, n-alkenes and n-alkyl chlorides. That is on the basis of their similar effect on properties of their respective chains. In addition, not only are the optimum values of y for these two series grouped in the density correlation, but also in the heat of vaporization correlation, where the following results were obtained:

n-alcohols	0.49 (0.43)
n-alkyl chlorides	0.25
n-acids	0.47 (0.38)
formate esters	0.63
n-alkyl benzenes	0.10 (0.65)

The values in parentheses indicate added data sets of Antoine constants or, in the case of n-alkyl benzene, higher pressure levels of prediction.

Admittedly these results do not show the same consistency as that demonstrated by the results reported by Kemme, however, the

grouping of the alcohol and acid groups is quite clear.

It would be well to note one other point. If one analyzes the results of this work and Kemme's work, one can easily see a progression of optimum values of y from the acid-alcohol grouping at 0.20 to the alkane-alkene-alkyl halide grouping at 0.60 to the larger end group alkyl benzene at 0.78. This progression seems to substantiate Kemme's suggestion of one value of y for homologous series in that different types of end grouped homologous series exhibit makedly different values of optimum, y.

Heat of Vaporization Correlation

Kemme (5) has suggested a single value of 0.675 as the power of the carbon number for determining the effective chain length parameter, x, in the heat of vaporization correlation after having studied the n-alkanes, n-alkenes, n-alkyl chlorides and n-alcohols. An examination of the results of this work based upon the limited available data presented in Appendix B suggests this is not the case for all series. Present work would preferably indicate the use of a common value for groups of homologous series as described above.

It may be recalled that the heat of vaporization expression was given in terms of three constants as follows:

$$E_V = A + Cx + Dx \ln P \qquad (25)$$

Kemme has suggested, and this work substantiates, that this equation will correlate the internal heat of vaporization of

an entire homologous series as a function of vapor pressure and carbon number. From the equation it can be easily seen that A may be defined as the heat of vaporization when the carbon number is zero. Kemme reported values of A for the series he investigated as follows:

n-alkanes	-304.91 cal./gm. mole (or essentially zero)
n-alkenes	125.43 cal./gm. mole
n-alkyl chlorides	3,228.6 cal./gm. mole
n-alcohols	7,341.2 cal./gm. mole

Kemme has said that the value of A for the n-alkanes can be assumed to be zero since the only end group to give rise to a heat of vaporization is a hydrogen atom. For alkenes A is a slight positive value and may be attributed to the effect of the double bond. For the alkyl chlorides the value of A is equal to the attractive energy of the Cl- group. The comparatively high value of A displayed by the alcohols reflects the effect of hydrogen bonding.

Kemme concludes that it is possible to obtain approximate additive values for the heat of vaporization for different organic groups. As a point of interest and further substantiation of this position the following presents the values of A determined in the course of this work:

n-alcohols	7,351 cal./gm. mole (7,585)
n-alkyl chlorides	3,759 cal./gm. mole
n-acids	7,037 cal./gm. mole (7,430)
n-esters formate	4,556 cal./gm. mole
n-alkyl benzenes	2,006 cal./gm. mole (755)

Here again the values in parentheses indicate additional data sets of Antoine constants or, in the case of n-alkyl benzene, higher pressure levels of prediction.

A comparison between the above values and those reported by Kemme indicates a remarkable duplication when one considers the variety in data utilized in this work. It can be seen that for the two series considered by both Kemme and this work, n-alkyl chlorides and n-alcohols, the values for A are virtually identical 3,228.6 versus 3,759 and 7,341.2 versus 7,351 respectively. This in itself says a great deal about the validity of the correlation. A further examination between the n-acids and the n-alcohols again points out the validity of grouping these series since the A values are 7,037 and 7,351 respectively and 7,430 and 7,585 respectively - reflecting the use of different data sets of Antoine constants in the correlation. With these results one can easily see that the effect of the acid and alcohol end groups are similar. Based upon this analysis it would also seem that the n-alkyl chlorides should be grouped with the n-alcohols and n-acids rather than with the n-alkanes and n-alkenes at least for the heat of vaporization correlation and perhaps for the density correlation.

As noted by Kemme the effect of a terminal group becomes smaller and smaller as the chain length increases. Thus the heat of vaporization of compounds with large carbon numbers in a given series approach the same value. This effect can be noted in all the series investigated in this work.

Conclusions

1. As concluded by Kemme and substantiated in this work the molal liquid density of a straight chain homologous series of organic compounds may be validly expressed as a function of vapor pressure and the number of carbon atoms, N, in the following form:

$$\ln (T \rho_l) = C + D \ln P + Ex + Fx \ln P$$

where $x = N^y$

and C, D, E, F and y are constants.

2. Homologous series of straight chain hydrocarbons may be grouped for purposes of establishing a value of y applicable to each group. This grouping should be done based upon relative degree of association of the end groups in the series under consideration. The value of y may be considered a measure of the spacial contribution of the end group under consideration.

3. The internal heats of vaporization of a straight chain homologous series of organic compounds may be validly expressed as a function of the vapor pressure and number of carbon atoms, N, in the following form:

$$Ev = A + Cx + Dx \ln P$$

where $x = N^y$

and A, C, D and y are constants.

4. The value of y for a group of straight chain homologous series is dependent on the degree of association of the end group under consideration.

5. The value of the constant A in the heat of vaporization equation may be considered a measure of the attractiveness of the end group under consideration and can be used to group the homologous series for purposes of establishing a common y.

6. A number of Antoine constants were catalogued and tabulated for future as well as present use.

7. Multi-linear regression computer programs presented by Kemme were converted and debugged for use on an IBM-360/65 system, using Fortran IV.

E_v = internal heat of vaporization, cal./gm. mole

f = free energy per molecule related to intramolecular freedoms

F = Helmholtz free energy

ΔH_v = external heat of vaporization, cal./gm. mole

k = Boltzmann constant

N = number of carbon atoms in a molecular chain

N_A = Avagadro's number

N_o = number of molecules in a system

P = vapor pressure mm Hg

R = gas constant

t = temperature, ^oC

T = absolute temperature, ^oK

T_b = normal boiling point, ^oK

v_g = volume per gaseous molecule

v_l = volume per liquid molecule

v_g' = molal volume of the gaseous phase

v_l' = molal volume of the liquid phase

V = volume of the system or lattice

x = number of consecutive cells

y = effective chain length power

z = coordination number

Z_g = gas compressibility factor

Z_l = liquid compressibility factor

ΔZ = difference between gas and liquid compressibility factors

ϵ = internal energy

μ = the chemical potential

ρ_l = liquid density, gm. mole/ml.

τ = cell volume

ψ = an increase in free energy.

APPENDIX

TABLE OF CONTENTS

APPENDIX A

Multi-Linear Regression of the Modified Kurata-Isida Heat of Vaporization Equation

Method Employed

The basis for this computation is available on page 278 of Volk (10). A complete set of equations describing the solution for the regression correlation of two independent variables by the method of Gaussian multipliers are presented. Volk also presents statistical parameters useful in the analysis of the correlation. This information together with the computer program presented here should describe the method employed for data correlation and output.

Required Input Data

The program is presented in IBM System 360, Fortran IV Language. The data input format is as indicated in the program. The required data input order must be as follows:

1. Listing of probability factors for a probability of deviation greater than t of 0.025.
2. Individual vapor pressure points (nine).
3. The number of compounds to be correlated.
4. The homologous series identification number.
5. Number of carbon atoms for each compound followed by.
6. The Antoine constants for each compound.
7. The effective chain length power to be used in the correlation.

NOMENCLATURE FOR THE MULTI-LINEAR REGRESSION OF THE MODIFIED KURATA-ISIDA HEAT OF VAPORIZATION CORRELATION

TTEST = Listing of Student's probability factors

PP = Vapor pressure

L = Number of compounds

SERIES = Homologous series identification number

CN = Number of carbon atoms

CODE = Compound identification number

A,B,C = Antoine constants

PW = Chain length power

AA,B1,B2 = Linearized equation constants

ALO = Lowest value of AA about 95% C.I.

B1LO = Lowest value of B1 about 95% C.I.

B2LO = Lowest value of B2 about 95% C.I.

AHI = Highest value of AA about 95% C.I.

B1HI = Highest value of B1 about 95% C.I.

B2HI = Highest value of B2 about 95% C.I.

SPC2 = Sum of squares of regression

R = Correlation coefficient

S2YES2 = Residual sum of squares

DFS2Y = Degrees of freedom

A,B,C = Modified Kurata-Isida equation constants

X1LV = Experimental heat of vaporization

CX1LV = Calculated heat of vaporization

GOOF = Error on heat of vaporization estimate

PCER = Per cent error on heat of vaporization estimate

```
//   EXEC   FORTGCLG,PARM.FORT='DECK,LIST,ID'
// EXEC FORTGCLG
//FORT.SYSIN DD *
C      V.J. VASTA JR.   FEBRUARY 9, 1968
C      MULTILINEAR REGRESSION OF THE KEMME-KREPS INTERNAL HEAT OF
C      VAPORIZATION-VAPOR PRESSURE-CARBON NUMBER CORRELATION.
C      LATENT HEATS GENERATED USING CLAPEYRON AND ANTOINE EQUATION
C      Z ESTIMATE USING FISHTINES METHOD, SEE I/EC VOL. 55 MAY 1963 PP49
C      REGRESSION METHOD FROM VOLK, PG. 278 (METHOD OF GAUSSIAN MULT.)
C
       DIMENSION          P(9, 20), PP(9),    C(20),    CN(20),
      1          TC(9, 20),          CODE(20), A(20),    B(20),
      2          XILV(9, 20),        X(20),    TTEST(34)
C
       DO         10 N = 1, 34
    10 READ       20, TTEST(N)
    20 FORMAT     ( F10.0 )
       DO         30 J = 1, 9
    30 READ       20, PP(J)
       READ       40, L
    40 FORMAT     ( I5 )
       READ       20, SERIES
       DO         60 K = 1, L
       READ       20, CN(K)
       READ       50, CODE(K), A(K), B(K), C(K)
    50 FORMAT     ( 4F10.0 )
       DO         60 J = 1, 9
       P(J, K) = PP(J)
       ZTERM   = ALOG ( P(J, K) ) * 0.43429
    60 TC(J, K) = ( B(K) / ( A(K) - ZTERM ) ) - ( C(K) )
       DO         190 K = 1, L
       DO         190 J = 1, 9
       TA      = TC(J, K) + 273.16
       TB      = TC(9, K) + 273.16
       TN      = TC(J, K)
       TR      = TA / TB
       IF         ( TR - .99 ) 80, 70, 70
    70 DZ      = .95
       GO TO      180
    80 IF         ( TR - .96 ) 100, 90, 90
    90 DZ      = .96
       GO TO      180
   100 IF         ( TR - .92 ) 120, 110, 110
   110 DZ      = .97
       GO TO      180
   120 IF         ( TR - .87 ) 140, 130, 130
   130 DZ      = .98
       GO TO      180
   140 IF         ( TR - .79 ) 160, 150, 150
   150 DZ      = .99
       GO TO      180
   160 IF         ( TR - .74 ) 170, 170, 170
   170 DZ      = 1.00
       GO TO      180
   180 R       = 1.987
       XLV     = ( ( 2.303 ) * ( R ) * ( TA ** 2.0 ) * ( B(K) ) * ( DZ ) )
      1            / ( ( TN + C(K) ) ** 2.0 )
   190 XILV(J, K) = XLV - DZ * R * TA
       EN      = 9 * L
```

```
200 READ      20, PW
    SY      = 0.0
    SX1     = 0.0
    SX2     = 0.0
    DO        210 K = 1, L
    X(K)    = CN(K) ** PW
    DO        210 J = 1, 9
    SY      = SY + XILV(J, K)
    SX1     = SX1 + X(K) * ALOG ( P(J, K) )
210 SX2     = SX2 + X(K)
    YBAR    = SY / EN
    X1BAR   = SX1 / EN
    X2BAR   = SX2 / EN
    SPY2    = 0.0
    SPYX1   = 0.0
    SPYX2   = 0.0
    SPX1X2  = 0.0
    S2X2    = 0.0
    S2X1    = 0.0
    DO        220 K = 1, L
    DO        220 J = 1, 9
    DELY    = XILV(J, K) - YBAR
    DELX1   = X(K) * ALOG ( P(J, K) ) - X1BAR
    DELX2   = X(K) - X2BAR
    DEL2X1  = DELX1 * DELX1
    DEL2X2  = DELX2 * DELX2
    DEL2Y   = DELY * DELY
    SPY2    = SPY2 + DEL2Y
    SPYX1   = SPYX1 + DELY * DELX1
    SPYX2   = SPYX2 + DELY * DELX2
    SPX1X2  = SPX1X2 + DELX1 * DELX2
    S2X2    = S2X2 + DEL2X2
220 S2X1    = S2X1 + DEL2X1
    SPXX2   = SPX1X2 * SPX1X2
    DENOM   = S2X1 * S2X2 - SPXX2
    B1      = ( SPYX1 * S2X2 - SPYX2 * SPX1X2 ) / DENOM
    B2      = ( SPYX2 * S2X1 - SPYX1 * SPX1X2 ) / DENOM
    AA      = YBAR - B1 * X1BAR - B2 * X2BAR
    SPC2    = B1 * SPYX1 + B2 * SPYX2
    R       = ( SPC2 / SPY2 ) ** 0.5
    S2YES2  = SPY2 - SPC2
    DFS2Y   = EN - 3.0
    F       = SQRT ( SPC2 ) / SQRT ( S2YES2 )
    S2YES   = S2YES2 / DFS2Y
    GAUS11  = S2X2 / DENOM
    GAUS22  = S2X1 / DENOM
    GAUS12  = SPX1X2 / DENOM
    S2B1    = S2YES * GAUS11
    S2B2    = S2YES * GAUS22
    SDB1    = SQRT ( S2B1 )
    SDB2    = SQRT ( S2B2 )
    N       = DFS2Y
    IF        ( N - 30 ) 230, 230, 240
230 GO TO     330
240 IF        ( N - 35 ) 250, 250, 260
250 N       = 30
    GO TO     330
260 IF        ( N - 50 ) 270, 270, 280
270 N       = 31
```

```
      GO TO    330
280   IF       ( N - 90 ) 290, 290, 300
290   N      = 32
      GO TO    330
300   IF       ( N - 150 ) 310, 310, 320
310   N      = 33
      GO TO    330
320   N      = 34
330   B1LO   = B1 - SDB1 * TTEST(N)
      B1H1   = B1 + SDB1 * TTEST(N)
      B2LO   = B2 - SDB2 * TTEST(N)
      B2H1   = B2 + SDB2 * TTEST(N)
      ALO    = YBAR - B1H1 * X1BAR - B2H1 * X2BAR
      AHI    = YBAR - B1LO * X1BAR - B2LO * X2BAR
      PRINT    340, SERIES, PW
340   FORMAT   ( 31HTHE LINEAR EQUATION FOR SERIES , F7.2, 3H IS, /, 5X,
     1          7HX=CN**,, F7.4, / )
      PRINT    350, AA, B1, B2
350   FORMAT   ( 6HINHV= , E12.6, 3H + , E12.6, 4HXLNP, 3H + , E12.6,
     1          1HX, / / )
      PRINT    360
360   FORMAT   ( / 5X, 36HTHE 95 PERCENT CONFIDENCE LIMITS ARE )
      PRINT    370, ALO, AHI
370   FORMAT   ( 5X, 3HA= , E14.8, 4H TO , E14.8 )
      PRINT    380, B1LO, B1H1
380   FORMAT   ( 5X, 4HB1= , E14.8, 4H TO , E14.8 )
      PRINT    390, B2LO, B2H1
390   FORMAT   ( 5X, 4HB2= , E14.8, 4H TO , E14.8, / )
      PRINT    400
400   FORMAT   ( 17X, 43HANALYSIS OF VARIANCE OF THE LINEAR EQUATION )
      PRINT    410
410   FORMAT   ( 17X, 43H-------------------------------------------, /
     1          )
      PRINT    420, EN
420   FORMAT   ( 18X, F6.0, 11HDATA POINTS / )
      PRINT    430, SPC2
430   FORMAT   ( 8X, 30HSUM OF SQUARES OF REGRESSION= , E14.8 )
      PRINT    440, R
440   FORMAT   ( 8X, 27HCORRELATION COEFFICIENT R= , F10.7 )
      PRINT    450, S2YES2, DFS2Y
450   FORMAT   ( 8X, 25HRESIDUAL SUM OF SQUARES= , E14.8, 5H FOR , F6.0,
     1          19H DEGREES OF FREEDOM )
      PRINT    460, F
460   FORMAT   ( 8X, 28HF TEST FOR SIGNIFICANCE, F= , F8.2 )
      PRINT    470, DFS2Y
470   FORMAT   ( 8X, 38HCONSULT VOLK PAGES 148-151, F2= 2,F1= , F6.0 )
      PRINT    480
480   FORMAT   ( 8X, 42HTO FIND PROBABILITY OF A LARGER VALUE OF F )
      PRINT    490, S2YES
490   FORMAT   ( 8X, 22HVARIANCE OF ESTIMATE= , E14.8 )
      PRINT    500, S2B1, S2B2
500   FORMAT   ( 8X, 35HVARIANCE OF REGRESSION COEFFICIENTS, / 12X,
     1          10HS**2(B1)= , E14.8 / 12X, 10HS**2(B2)= , E14.8, / / )
      PRINT    510
510   FORMAT   ( / / / 5X, 29HTHE KEMME-KREPS CONSTANTS ARE )
      PRINT    520, AA, B1, B2
520   FORMAT   ( / 10X, 3HA= , E14.8, / 10X, 3HB= , E14.8, / 10X, 3HC= ,
     1          E14.8 )
```

```
      PRINT     530
  530 FORMAT    ( / / /, 2X,
     1           48HERROR ANALYSIS OF THE INT. HEAT OF VAP. ESTIMATE )
      BIG     = 0.0
      SUMPE   = 0.0
      M10     = 0.0
      M5      = 0.0
      PRINT     540
  540 FORMAT    ( 2X,
     1           69HTEMP C    INHV XP    INHV CAL    ERROR      PC ERR    Z
     2  PRESSURE MM HG, / )
      SUMS    = 0.0
      DO        620 K = 1, L
      PRINT     550, CODE(K)
  550 FORMAT    ( 23X, 9HCOMPOUND , F7.2  )
      DO        620 J = 1, 9
      CXILV   = AA + B1 * X(K) * ALOG ( P(J, K) ) + B2 * X(K)
      GOOF    = CXILV - XILV(J, K)
      PCER    = GOOF * 100.0 / XILV(J, K)
      Z       = XILV(J, K) / CXILV
      ABSER   = ABS ( PCER )
      IF        ( ABSER - 5.0 ) 560, 570, 570
  560 M5      = M5 + 1
      GO TO     590
  570 IF        ( ABSER - 10.0 ) 590, 590, 580
  580 M10     = M10 + 1
  590 SUMPE   = SUMPE + ABSER
      SUMS    = SUMS + GOOF
      PRINT     600, TC(J, K), XILV(J, K), CXILV, GOOF, PCER, Z, P(J, K)
  600 FORMAT    ( 2X, F6.1, 2X, F10.3, 1X, F10.3, 1X, F9.3, 1X, F7.2, 1X,
     1           F7.4, 1X, F8.2 )
      IF        ( ABSER - BIG ) 620, 620, 610
  610 BIG     = ABSER
  620 CONTINUE
      AVERR   = SUMPE / EN
      PRINT     630, AVERR
  630 FORMAT    ( / 12X, 24HAVERAGE ABSOLUTE ERROR= , F10.5, 8H PERCENT )
      PRINT     640, BIG
  640 FORMAT    ( 12X, 24HMAXIMUM ABSOLUTE ERROR= , F10.5, 8H PERCENT )
      GOOD    = M5
      BAD     = M10
      APOO    = BAD / EN * 100.0
      AWOW    = GOOD / EN * 100.0
      PRINT     650, AWOW, APOO
  650 FORMAT    ( 2X, F6.1, 35H PERCENT OF ERRORS UNDER 5 PERCENT,, F5.1,
     1           24H PERCENT OVER 10 PERCENT / )
      SD      = SQRT ( SUMS / ( EN - 1.0 ) )
      ENN     = EN - 1.0
      N       = ENN
      IF        ( N - 30 ) 660, 660, 670
  660 GO TO     760
  670 IF        ( N - 35 ) 680, 680, 690
  680 N       = 30
      GO TO     760
  690 IF        ( N - 50 ) 700, 700, 710
  700 N       = 31
      GO TO     760
  710 IF        ( N - 60 ) 720, 720, 730
  720 N       = 32
```

```
      GO TO     760
730   IF        ( N - 150 ) 740, 740, 750
740   N       = 33
      GO TO     760
750   N       = 34
760   CONTINUE
      RANGE   = SD + TTEST(N)
      PRINT     770
770   FORMAT    ( 2X,
     1           51H95 PERCENT CONFIDENCE RANGE OF HEAT OF VAPORIZATION
      PRINT     780, RANGE
780   FORMAT    ( 8X, 7HD +OR- , F7.4 )

      PRINT     790
790   FORMAT    ( 25X, 33H----------CASE COMPLETE---------- / / / )
      GO TO     200
      END
```

Multi-Linear Regression of the Kemme-Kreps Density Equation

Method Employed

The regression correlation is solved using the equations shown in Volk (10) pages 262 and 287. The program is presented in IBM System 360, Fortran IV Language. To facilitate the computation of the variables to the required degree of significance the program is written having three sub-routines. The sub-routines are identified as ADDD, BDDD and CDDD.

Required Input Data

The data input format is as indicated in the program. The required data input order must be as follows:

1. Listing of probability factors for a probability of deviation greater than t of 0.025.
2. The homologous series identification number.
3. The number of compounds to be correlated.
4. The Antoine constants for each compound.
5. The number of carbon atoms, molecular weight and the number of data points for each compound.
6. The density-temperature data for each compound.
7. The effective chain length power to be used in the correlation.
8. Point by point error analysis, yes or no indicated by 2 or 1 respectively.

NOMENCLATURE FOR THE MULTI-LINEAR REGRESSION OF THE KEMME-KREPS DENSITY EQUATION

TTEST = Listing of Student's probability factors

CHOICE = Variable to indicate whether a point by point error analysis is to be carried out

SERIES = Homologous series identification number

K = Number of compounds

CODE = Compound identification number

AA,BB,CC = Antoine constants

CN = Number of carbon atoms

W = Molecular weight

EN = Number of data points per compound

TC = Temperature

TERM = Density

PW = Chain length power

A = Constants for the Kemme-Kreps equation

B1 = Constants for the Kemme-Kreps equation

B2 = Constants for the Kemme-Kreps equation

B3 = Constants for the Kemme-Kreps equation

SEN = Total number of data points

SPC2 = Sum of squares of regression

R = Correlation coefficient

S2YES2 = Residual sum of squares

DFS2Y = Degrees of freedom

GOOF = Error on density estimate

PCER = Per cent error on density estimate

AVERR = Average absolute error

BIG = Maximum absolute error

```
// EXEC FORTGCLG,PARM.FORT='DECK,LIST,MAP,ID'
//FORT.SYSIN   DD *
C
C      V.J. VASTA JR.   FEBRUARY 9, 1968
C      MUTILINEAR REGRESSION OF THE MODIFIED KURATA-ISIDA EQUATION
C      RELATING VAPOR PRESSURE AND LIQUID DENSITY.  FOR AN HOMO. SERIES
C      PROGRAM EMPLOYS THREE INDEPENDENT VARIABLES
C      DATA IN FORM AS FOLLOWS  (FLOATING POINT VARIABLES)
C       34 T TEST POINTS (ALREADY AT END OF PROGRAM)
C       SERIES NO.
C       NO. OF COMPOUNDS
C       COMPOUND CODE, ANTOINE A,B, AND C, CONSTANTS.
C       NO. OF CARBON ATOMS, MOLECULAR WGT., NO. OF DATA POINTS.
C       TEMP. C., DENSITY, GM/ML.
C
      DIMENSION          AA(20),   BB(20),   CC(20),   CN(20),   W(20),
     1          EN(20),   TC(20, 12),          TA(20, 12),
     2          DM(20, 12),          P(20, 12),          X(20),
     3          TERM(20, 12),        TTEST(34)
C
      COMMON    AA,       BB,       CC,       CN,       W,        EN,
     1          TC,       TA,       DM,       P,        X,        TERM,
     2          TTEST,    SERIES,   K,        SEN,      N,        SY,
     3          SX1,      SX2,      SX3,      X1,       X2,       YBAR,
     4          X1BAR,    X2BAR,    X3BAR,    SPY2,     SPYX2,    SPYX3,
     5          SPYX1,    SPX1X2,   SPX2X3,   SPX1X3,   SP2X1,    SP2X2,
     6          SP2X3,    DELY,     DELX1,    DELX2,    DELX3,    DEL2Y,
     7          E,        Y,        Z,        S,        R,        T,
     8          U,        Q,        F,        B1,       B2,       B3,
     9          A,        SPC2,     S2YES2,   DFS2Y
      COMMON    D,        BIG,      SUMPE,    M10,      M5,       SUMS,
     1          PXP,      GOOF,     PCER,     ABSER,    AVERR,    GOOD,
     2          BAD,      APOO,     AWOW,     SD,       ENN,      RANGE,
     3          S2YES,    B,        C,        DXP,      PW,       CHOICE,
     4          PASS
C
      PASS   = 0.0
   10 IF        (PASS .GT.0.0) GO TO 120
      DO        20 N = 1, 34
   20 READ      30, TTEST(N)
   30 FORMAT    ( F7.4 )
   40 READ      50, SERIES
   50 FORMAT    ( F5.1 )
      READ      60, K
   60 FORMAT    (I2)
      SEN    = 0
      DO        110 L = 1, K
      READ      70, CODE, AA(L), BB(L), CC(L)
   70 FORMAT    ( F7.1, F10.5, F10.5, F10.5 )
      READ      80, CN(L), W(L), EN(L)
   80 FORMAT    ( F4.1, F10.5, F10.5 )
      N      = EN(L)
      DO        100 J = 1, N
      READ      90, TC(L, J), TERM(L, J)
   90 FORMAT    ( F7.1, F7.6 )
      TA(L, J) = TC(L, J) + 273.16
      DM(L, J) = TERM(L, J) / W(L)
  100 P(L, J) = EXP ( ( AA(L) - BB(L) / ( TC(L, J) + CC(L) ) ) * 2.30259
     1          )
```

```
  110 SEN     = SEN + EN(L)
  120 READ      (5,130,END=200) PW
  130 FORMAT    ( F10.7 )
      READ      140, CHOICE
  140 FORMAT    ( F10.7 )
      TERM(L, J) = 0.0
      SY      = 0.0
      SX1     = 0.0
      SX2     = 0.0
      SX3     = 0.0
      DO        160 L = 1, K
      N       = EN(L)
      X(L)    = CN(L) ** PW
      DO        150 J = 1, N
      TERM(L, J) = ALOG ( TA(L, J) * DM(L, J) )
      SY      = SY + TERM(L, J)
      X1      = ALOG ( P(L, J) )
      SX1     = SX1 + X1
      X2      = X(L) * ALOG ( P(L, J) )
      SX2     = SX2 + X2
  150 SX3     = SX3 + X(L)
  160 CONTINUE
      YBAR    = SY / SEN
      X1BAR   = SX1 / SEN
      X2BAR   = SX2 / SEN
      X3BAR   = SX3 / SEN
      SPY2    = 0.0
      SPYX1   = 0.0
      SPYX2   = 0.0
      SPYX3   = 0.0
      SPX1X2  = 0.0
      SPX2X3  = 0.0
      SPX1X3  = 0.0
      SP2X1   = 0.0
      SP2X2   = 0.0
      SP2X3   = 0.0
  170 CALL      ADDD
      CALL      BDDD
      CALL      CDDD
      GO TO 10
  200 STOP
      END
C
      SUBROUTINE  ADDD
      DIMENSION           AA(20),   BB(20),   CC(20),   CN(20),   W(20),
     1          EN(20),   TC(20, 12),         TA(20, 12),
     2          DM(20, 12),         P(20, 12),          X(20),
     3          TERM(20, 12),       TTEST(34)
C
      COMMON    AA,       BB,       CC,       CN,       W,        EN,
     1          TC,       TA,       DM,       P,        X,        TERM,
     2          TTEST,    SERIES,   K,        SEN,      N,        SY,
     3          SX1,      SX2,      SX3,      X1,       X2,       YBAR,
     4          X1BAR,    X2BAR,    X3BAR,    SPY2,     SPYX2,    SPYX3,
     5          SPYX1,    SPX1X2,   SPX2X3,   SPX1X3,   SP2X1,    SP2X2,
     6          SP2X3,    DELY,     DELX1,    DELX2,    DELX3,    DEL2Y,
     7          E,        Y,        Z,        S,        R,        T,
     8          U,        Q,        F,        B1,       B2,       B3,
     9          A,        SPC2,     S2YES2,   DFS2Y
```

```
      .COMMON   D,        BIG,      SUMPE,    M10,      M5,       SUMS,
     1          PXP,      GOOF,     PCER,     ABSER,    AVERR,    GOOD,
     2          BAD,      APOO,     AWOW,     SD,       ENN,      RANGE,
     3          S2YES,    B,        C,        DXP,      PW,       CHOICE,
     4          PASS
C
      DO        180 L = 1, K
      N       = EN(L)
      DO        170 J = 1, N
      DELY    = TERM(L, J) - YBAR
      DELX1   = ALOG ( P(L, J) ) - X1BAR
      DELX2   = ( X(L) * ALOG ( P(L, J) ) ) - X2BAR
      DELX3   = X(L) - X3BAR
      DEL2Y   = DELY * DELY
      SPY2    = SPY2 + DEL2Y
      SPYX1   = SPYX1 + DELY * DELX1
      SPYX2   = SPYX2 + DELY * DELX2
      SPYX3   = SPYX3 + DELY * DELX3
      SPX1X2  = SPX1X2 + DELX1 * DELX2
      SPX2X3  = SPX2X3 + DELX2 * DELX3
      SPX1X3  = SPX1X3 + DELX1 * DELX3
      SP2X1   = SP2X1 + DELX1 * DELX1
      SP2X2   = SP2X2 + DELX2 * DELX2
  170 SP2X3   = SP2X3 + DELX3 * DELX3
  180 CONTINUE
      E       = SP2X1
      Y       = SPX1X2
      Z       = SPX1X3
      S       = SPX2X3
      R       = SP2X2
      T       = SP2X3
      U       = SPYX1
      Q       = SPYX2
      F       = SPYX3
      B1      = ( ( ( ( Q * S ) - ( F * R ) ) * ( ( Z * R ) - ( S * Y ) )
     1            ) - ( ( ( U * R ) - ( Q * Y ) ) * ( ( S * S ) - ( R * T
     2            ) ) ) ) / ( ( ( ( Y * S ) - ( Z * R ) ) * ( ( Z * R ) -
     3            ( S * Y ) ) ) - ( ( ( E * R ) - ( Y * Y ) ) * ( ( S * S
     4            ) - ( R * T ) ) ) )
      B2      = ( ( ( ( U * Y ) - ( Q * E ) ) * ( ( S * Z ) - ( T * Y ) )
     1            ) - ( ( ( Q * Z ) - ( F * Y ) ) * ( ( Z * Y ) - ( S * E
     2            ) ) ) ) / ( ( ( ( Y * Y ) - ( R * E ) ) * ( ( S * Z ) -
     3            ( T * Y ) ) ) - ( ( ( R * Z ) - ( S * Y ) ) * ( ( Z * Y
     4            ) - ( S * E ) ) ) )
      B3      = ( ( ( ( U * Y ) - ( Q * E ) ) * ( ( R * Z ) - ( S * Y ) )
     1            ) - ( ( ( Q * Z ) - ( F * Y ) ) * ( ( Y * Y ) - ( R * E
     2            ) ) ) ) / ( ( ( ( Z * Y ) - ( S * E ) ) * ( ( R * Z ) -
     3            ( S * Y ) ) ) - ( ( ( Y * Y ) - ( R * E ) ) * ( ( S * Z
     4            ) - ( T * Y ) ) ) )
      A       = ( YBAR ) - ( B1 * X1BAR ) - ( B2 * X2BAR ) - ( B3 * X3BAR
     1            )
      SPC2    = ( B1 * U ) + ( B2 * Q ) + ( B3 * F )
      S2YES2  = SPY2 - SPC2
      DFS2Y   = SEN - 3.0
      R       = ( SPC2 / SPY2 ) ** 0.5
      F       = SQRT ( SPC2 ) / SQRT ( S2YES2 )
      S2YES   = S2YES2 / DFS2Y
      RETURN
      END
```

```
C
      SUBROUTINE  BDDD
      DIMENSION           AA(20),   BB(20),   CC(20),   CN(20),   W(20),
     1          EN(20),   TC(20, 12),         TA(20, 12),
     2          DM(20, 12),         P(20, 12),          X(20),
     3          TERM(20, 12),       TTEST(34)
C
      COMMON    AA,       BB,       CC,       CN,       W,        EN,
     1          TC,       TA,       DM,       P,        X,        TERM,
     2          TTEST,    SERIES,   K,        SEN,      N,        SY,
     3          SX1,      SX2,      SX3,      X1,       X2,       YBAR,
     4          X1BAR,    X2BAR,    X3BAR,    SPY2,     SPYX2,    SPYX3,
     5          SPYX1,    SPX1X2,   SPX2X3,   SPX1X3,   SP2X1,    SP2X2,
     6          SP2X3,    DELY,     DELX1,    DELX2,    DELX3,    DEL2Y,
     7          E,        Y,        Z,        S,        R,        T,
     8          U,        Q,        F,        B1,       B2,       B3,
     9          A,        SPC2,     S2YES2,   DFS2Y
      COMMON    D,        BIG,      SUMPE,    M10,      M5,       SUMS,
     1          PXP,      GOOF,     PCER,     ABSER,    AVERR,    GOOD,
     2          BAD,      APOO,     AWOW,     SD,       ENN,      RANGE,
     3          S2YES,    B,        C,        DXP,      PW,       CHOICE,
     4          PASS
C
      PRINT     190, SERIES
  190 FORMAT    ( 41HTHE LINEAR EQUATION FOR THE HOMO. SERIES , F6.1,
     1           3H IS )
      PRINT     200, A, B1, B2, B3
  200 FORMAT    ( / / 2X, 11HLN(TA*DM)= , E14.8, 1H+, E14.8, 8HLN(P) + ,
     1           / E14.8, 9HXLN(P) + , E14.8, 1HX / / )
      PRINT     210
  210 FORMAT    ( 17X, 43HANALYSIS OF VARIANCE OF THE LINEAR EQUATION )
      PRINT     220
  220 FORMAT    ( 17X, 43H------------------------------------------- / )
      PRINT     230, SEN, PW
  230 FORMAT    ( 18X, F6.0, 11HDATA POINTS /, 6HX=CN**, F10.7, / )
      PRINT     240, SPC2
  240 FORMAT    ( 8X, 3CHSUM OF SQUARES OF REGRESSION= , E14.8 )
      PRINT     250, R
  250 FORMAT    ( 8X, 27HCORRELATION COEFFICIENT R= , F10.7 )
      PRINT     260, S2YES2, DFS2Y
  260 FORMAT    ( 8X, 25HRESIDUAL SUM OF SQUARES= , F10.7, 5H FOR , F6.0,
     1           18HDEGREES OF FREEDOM )
      PRINT     270, F
  270 FORMAT    ( 8X, 28HF TEST FOR SIGNIFICANCE, F= , F8.2 )
      PRINT     280, DFS2Y
  280 FORMAT    ( 8X, 38HCONSULT VOLK PAGES 148-151, F2= 2,F1= , F6.0 )
      PRINT     290
  290 FORMAT    ( 8X, 42HTO FIND PROBABILITY OF A LARGER VALUE OF F )
      PRINT     300, S2YES
  300 FORMAT    ( 8X, 22HVARIANCE OF ESTIMATE= , E14.8 )
      PRINT     310
  310 FORMAT    ( / / / 5X, 23HTHE KEMME CONSTANTS ARE )
      B       = B1
      C       = B2
      D       = B3
      PRINT     320, A, B, C, D
  320 FORMAT    ( / 10X, 3HA= , E14.8, / 10X, 3HB= , E14.8, / 10X, 3HC= ,
     1           E14.8, / 10X, 3HD= , E14.8 )
      IF        ( CHOICE - 1.0 ) 360, 360, 330
```

```
  330 PRINT    340
  340 FORMAT   ( / / / 2X, 38HERROR ANALYSIS OF THE DENSITY ESTIMATE,
     1          )
      BIG     = 0.0
      SUMPE   = 0.0
      M10     = 0
      M5      = 0
      PRINT    350
  350 FORMAT   ( 2X,
     1          70HTEMP C   DEN XP  DEN CAL   ERROR   PC ERR     Z
     2   PRESSURE MM HG, / )
      SUMS    = 0.0
  360 CONTINUE
      RETURN
      END
C
      SUBROUTINE  CDDD
      DIMENSION          AA(20),   BB(20),   CC(20),   CN(20),   W(20),
     1          EN(20),   TC(20, 12),          TA(20, 12),
     2          DM(20, 12),          P(20, 12),          X(20),
     3          TERM(20, 12),        TTEST(34)
C
      COMMON   AA,        BB,        CC,        CN,        W,         EN,
     1         TC,        TA,        DM,        P,         X,         TERM,
     2         TTEST,     SERIES,    K,         SEN,       N,         SY,
     3         SX1,       SX2,       SX3,       X1,        X2,        YBAR,
     4         X1BAR,     X2BAR,     X3BAR,     SPY2,      SPYX2,     SPYX3,
     5         SPYX1,     SPX1X2,    SPX2X3,    SPX1X3,    SP2X1,     SP2X2,
     6         SP2X3,     DELY,      DELX1,     DELX2,     DELX3,     DEL2Y,
     7         E,         Y,         Z,         S,         R,         T,
     8         U,         Q,         F,         B1,        B2,        B3,
     9         A,         SPC2,      S2YES2,    DFS2Y
      COMMON   D,         BIG,       SUMPE,     M10,       M5,        SUMS,
     1         PXP,       GOOF,      PCER,      ABSER,     AVERR,     GOOD,
     2         BAD,       APOO,      AWOW,      SD,        ENN,       RANGE,
     3         S2YES,     B,         C,         DXP,       PW,        CHOICE,
     4         PASS
C
      IF         ( CHOICE - 1.0 ) 360, 360, 330
  330 DO         450 L = 1, K
      N       = EN(L)
      DO         440 J = 1, N
      D       = B3
      DXP     = ( ( EXP ( A + B * ALOG ( P(L, J) ) + C * X(L) * ALOG
     1            ( P(L, J) ) + D * X(L) ) ) / ( TA(L, J) ) ) * ( W(L) )
      D       = DM(L, J) * W(L)
      GOOF    = DXP - D
      PCER    = GOOF * 100.0 / D
      Z       = D / DXP
      ABSER   = ABS ( PCER )
      IF         ( ABSER - 5.0 ) 380, 390, 390
  380 M5      = M5 + 1
      GO TO      410
  390 IF         ( ABSER - 10.0 ) 410, 410, 400
  400 M10     = M10 + 1
  410 SUMPE   = SUMPE + ABSER
      SUMS    = SUMS + GOOF
      PRINT      420, TC(L, J), D, DXP, GOOF, PCER, Z, P(L, J)
  420 FORMAT   ( 2X, F6.1, 2X, F8.5, 1X, F8.5, 1X, F8.5, 1X, F7.2, 2X,
```

```
     1          F6.3, 5X, F8.2 )
      IF        ( ABSER - BIG ) 440, 440, 430
430 BIG     = ABSER
440 CONTINUE
450 CONTINUE
     AVERR  = SUMPE / SEN
     PRINT     460, AVERR
460 FORMAT    ( / 12X, 24HAVERAGE ABSOLUTE ERROR= , F10.5, 8H PERCENT
     PRINT     470, BIG
470 FORMAT    ( 12X, 24HMAXIMUM ABSOLUTE ERROR= , F10.5, 8H PERCENT
     GOOD   = M5
     BAD    = M10
     APOO   = BAD / SEN * 100.0
     AWOW   = GOOD / SEN * 100.0
     PRINT     480, AWOW, APOO
480 FORMAT    ( 2X, F6.1, 35H PERCENT OF ERRORS UNDER 5 PERCENT,, F5.1,
    1           24H PERCENT OVER 10 PERCENT / )
     SD     = SQRT ( SUMS / ( SEN - 1.0 ) )
     ENN    = SEN - 1.0
     N      = ENN
     IF        ( N - 30 ) 490, 490, 500
490 GO TO     590
500 IF        ( N - 35 ) 510, 510, 520
510 N       = 30
     GO TO     590
520 IF        ( N - 50 ) 530, 530, 540
530 N       = 31
     GO TO     590
540 IF        ( N - 60 ) 550, 550, 560
550 N       = 32
     GO TO     590
560 IF        ( N - 150 ) 570, 570, 580
570 N       = 33
     GO TO     590
580 N       = 34
590 CONTINUE
     RANGE  = SD * TTEST(N)
     PRINT     600
600 FORMAT    ( 2X, 48H95 PERCENT CONFIDENCE RANGE OF VAPOR PRESSURE IS
    1           )
     PRINT     610, RANGE
610 FORMAT    ( 8X, 7HD +OR- , F7.4 )
360 PRINT     630
630 FORMAT    ( 15X, 33H----------CASE COMPLETE---------- / / / )
     PASS   = 2.0
     RETURN
     END
```

APPENDIX B

LITERATURE DENSITY DATA FOR ACIDS

Temp. °C	Density gm/ml	Literature Source
	FORMIC ACID	
		CN = 1
15	1.2265	(8)
25	1.2141	(8)
30	1.2078	(8)
40	1.1954	(8)
	ACETIC ACID	
		CN = 2
20	1.0491	(8)
30	1.0392	(8)
40	1.0284	(8)
50	1.0175	(8)
60	1.0060	(8)
70	0.9948	(8)
80	0.9835	(8)
90	0.9718	(8)
100	0.9599	(8)
110	0.9483	(8)
120	0.9362	(8)
130	0.9235	(8)
140	0.9091	(8)
150	0.8963	(8)
160	0.8829	(8)
170	0.8694	(8)
	PROPIONIC ACID	
		CN = 3
0	1.0150	(8)
15	0.9987	(8)
20	0.9826	(8)
	h-BUTYRIC ACID	
		CN = 4
0	0.9777	(8)
10	0.9682	(8)
20	0.9580	(8)
30	0.9479	(8)
40	0.9377	(8)
50	0.9274	(8)
58.8	0.9198	(8)
67.4	0.9113	(8)
	n-VALERIC ACID	
		CN = 5
0	0.9574	(8)
15	0.9437	(8)
19.1	0.9397	(8)
25	0.9348	(8)
30	0.9302	(8)
	n-CAPROIC ACID	
		CN = 6
0	0.9443	(8)
15	0.9314	(8)
25	0.9230	(8)
30	0.9183	(8)
80	0.8751	(8)
	n-HEPTANOIC ACID	
		CN = 7
0	0.9345	(8)
15	0.9222	(8)
30	0.9099	(8)
80	0.8670	(8)
	n-CAPRYLIC ACID	
		CN = 8
20	0.9088	(8)
30	0.9009	(8)
80	0.8615	(8)

LITERATURE DENSITY DATA FOR ACIDS

Temp. °C	Density gm/ml	Literature Source
	n-CAPRIC ACID	
		CN = 10
35.05	0.8884	(8)
40.0	0.8858	(8)
50.17	0.8773	(8)
80.0	0.8531	(8)
	n-LAURIC ACID	
		CN = 12
45.1	0.8744	(8)
50.25	0.8707	(8)
70.0	0.8573	(8)
78.5	0.8495	(8)
80.0	0.8477	(8)
82.1	0.8475	(8)
	n-MYRISTIC ACID	
		CN = 14
60	0.8584	(8)
70	0.8533	(8)
80	0.8439	(8)
90	0.8394	(8)
	n-PALMITIC ACID	
		CN = 16
70	0.8487	(8)
80	0.8414	(8)
90	0.8347	(8)
	n-MARGARIC ACID	
		CN = 17
90.6	0.8355	(8)
100.7	0.8282	(8)
110.2	0.8213	(8)
129.0	0.8092	(8)
135.7	0.8039	(8)
146.5	0.7961	(8)
	n-STEARIC ACID	
		CN = 18
80	0.8390	(8)

LITERATURE DENSITY DATA FOR ESTERS-FORMATE

METHYL FORMATE

CN = 2

Temp. °C	Density gm/ml	Literature Source
0	1.0032	(8)
20	0.9745	(8)
40	0.9447	(8)
60	0.9133	(8)
80	0.8803	(8)
100	0.8452	(8)
120	0.8070	(8)
140	0.7638	(8)
160	0.7136	(8)
180	0.6521	(8)
200	0.5658	(8)
210	0.4857	(8)

ETHYL FORMATE

CN = 3

Temp. °C	Density gm/ml	Literature Source
0	0.9480	(8)
20	0.9226	(8)
40	0.8963	(8)
60	0.8689	(8)
80	0.8409	(8)
100	0.8112	(8)
120	0.7796	(8)
140	0.7448	(8)
160	0.7058	(8)
180	0.6610	(8)
200	0.6066	(8)
220	0.5290	(8)

n-PROPYL FORMATE

CN = 4

Temp. °C	Density gm/ml	Literature Source
0	0.9287	(8)
20	0.9058	(8)
40	0.8827	(8)
60	0.8588	(8)
80	0.8341	(8)
100	0.8080	(8)
120	0.7811	(8)
140	0.7523	(8)
160	0.7209	(8)
180	0.6873	(8)
200	0.6487	(8)
220	0.6024	(8)
240	0.5438	(8)
260	0.4404	(8)

n-HEXYL FORMATE

CN = 7

Temp. °C	Density gm/ml	Literature Source
0	0.8996	(8)
15	0.8859	(8)
30	0.8722	(8)

n-HEPTYL FORMATE

CN = 8

Temp. °C	Density gm/ml	Literature Source
0	0.8959	(8)
15	0.8828	(8)
30	0.8697	(8)

n-OCTYL FORMATE

CN = 9

Temp. °C	Density gm/ml	Literature Source
0	0.8912	(8)
15	0.8756	(8)
30	0.8659	(8)

LITERATURE DENSITY DATA FOR ALKYL-BENZENE

Temp. °C	Density gm/ml	Literature Source
	TOLUENE	
		CN = 7
0	0.8855	(8)
20	0.8670	(8)
30	0.8577	(8)
46.3	0.8425	(8)
56.4	0.8328	(8)
80	0.8102	(8)
90	0.8023	(1)
100	0.7931	(1)
110	0.7838	(1)
126.85	0.7622	(8)
	ETHYL BENZENE	
		CN = 8
0	0.8846	(8)
20	0.8671	(8)
30	0.8581	(8)
45.5	0.8441	(8)
50	0.8405	(1)
59.95	0.8314	(8)
79.7	0.8137	(8)
90	0.8041	(1)
97.6	0.7970	(8)
125.9	0.7702	(8)
	n-PROPYL BENZENE	
		CN = 9
0	0.8786	(8)
20	0.8618	(8)
38.3	0.8469	(8)
50	0.8371	(1)
62.75	0.8264	(8)
76.1	0.8148	(8)
99.55	0.7942	(8)
130	0.7661	(8)

Temp. °C	Density gm/ml	Literature Source
	n-BUTYL BENZENE	
		CN = 10
0	0.8761	(8)
15	0.8642	(8)
30	0.8522	(8)
	n-AMYL BENZENE	
		CN = 11
0	0.8741	(8)
15	0.8626	(8)
30	0.8510	(8)
	n-HEXYL BENZENE	
		CN = 12
0	0.8753	(8)
15	0.8639	(8)
30	0.8526	(8)

APPENDIX C

Antoine Constants

Series Name: Alcohols

Pressure Range (mm Hg) - Top: .99 E 49
Bottom: .99 E-49

Series Code: 100

Compound Code	Carbon Number	Antoine Constants A	B	C
101	1	7.9483878	1513.6744	233.83513
102	2	7.8868180	1474.5130	216.24497
103	3	-	-	-
104	4	-	-	-
105	5	7.2612042	1351.4537	171.05659
106	6	8.2282293	1990.1848	215.72796
107	7	6.0283805	859.40935	95.262477
108	8	7.0195740	1417.8615	147.45440
109	9	-	-	-
110	10	6.5596629	1269.1700	113.34668
111	11	-	-	-
112	12	7.5012027	1969.9518	164.60153

Antoine Constants

Series Name: Alcohols

Pressure Range (mm Hg) - Top: 10,000
Bottom: 30

Series Code: 100

Compound Code	Carbon Number	Antoine Constants A	B	C
101	1	7.4912101	1289.0680	214.16597
102	2	7.8755081	1469.4570	215.87313
103	3	7.5233097	1313.1289	185.63462
104	4	7.3179656	1288.0088	172.54901
104 10,000 1	4	7.4709858	1378.4008	182.40961
105	5	-	-	-
106	6	6.7121907	1107.9837	131.91133
107	7	7.0719437	1377.1609	152.57215
108	8	6.7842523	1279.9645	132.61339
109	9	-	-	-
110	10	6.6610683	1317.3881	117.62246
111	11	-	-	-
112	12	6.8758781	1555.2222	125.54293

Antoine Constants

Series Name: Alcohols

Pressure Range (mm Hg) - Top: 30 30

Bottom: 0 .99 E-49

Series Code: 100

Compound Code	Carbon Number	Antoine Constants A	B	C
101	1	-	-	-
102	2	-	-	-
103 30 0	3	4.3671591	356.20219	91.738273
104	4	-	-	-
105	5	-	-	-
106 30 .99 E-49	6	3.8920603	347.43009	61.415131
107 30 .99 E-49	7	3.0117408	131.91924	-8.8842963
108 30 .99 E-49	8	1.7393029	134.12520	-69.627667
109	9	-	-	-
110 30 .99 E-49	10	5.8060711	948.42137	82.658769
111	11	-	-	-
112 30 .99 E-49	12	8.1454781	2412.7350	199.33486

Antoine Constants

Series Name: Ketones

Pressure Range (mm Hg) - Top: .99 E 49
Bottom: .99 E-49

Series Code: 200

Compound Code	Carbon Number	Antoine Constants A	B	C
203 40,000 1.0	3	7.3290819	1393.6986	255.6653
203 40,000 760	3	8.1353802	1999.7485	324.31449
203 10,000 30	3	8.7825170	2274.7940	329.12952
203 30 0	3	1.8673504	25.829090	72.309425
204 .99 E 49 .99 E-49	4	4.8036105	348.03006	98.398489

Antoine Constants

Series Name: Alkyl Halides (Br)

Pressure Range (mm Hg) - Top: .99 E 49

Bottom: .99 E-49

Series Code: 300

Compound Code	Carbon Number	Antoine Constants A	B	C
301	1	7.1098600	1053.6110	245.62793
304	4	7.0636314	1367.9628	225.62394

Antoine Constants

Series Name: Alkyl Halides (CL)

Pressure Range (mm Hg) - Top: .99 E 49
Bottom: .99 E-49

Series Code: 400

Compound Code	Carbon Number	Antoine Constants A	B	C
401	1	6.8154590	837.15998	236.81049
402	2	6.6472076	886.55172	222.84720
403	3	-	-	-
404	4	6.7878357	1152.9208	216.43724
405	5	7.3672560	1588.1549	246.08688

Antoine Constants

Series Name: Alkyl Halides (I)

Pressure Range (mm Hg) - Top: .99 E 49

Bottom: .99 E-49

Series Code: 600

Compound Code	Carbon Number	Antoine Constants A	B	C
602	2	7.1822542	1353.4026	242.26546

Antoine Constants

Series Name: Acids

Pressure Range (mm Hg) - Top: .99 E 49

Bottom: .99 E-49

Series Code: 700

Compound Code	Carbon Number	Antoine Constants A	B	C
701	1	5.8130496	773.53359	159.00956
702	2	7.7493024	1764.2843	244.12015
703	3	-	-	-
704	4	-	-	-
705	5	-	-	-
706	6	8.0094341	2028.2383	191.25324
707	7	7.8355832	1988.4673	178.73134
708	8	7.7298590	1957.8115	165.62545
709	9	7.7602591	2047.0549	164.81404
710	10	7.5289781	1933.0015	146.36516
711	11	7.6432276	2064.2072	150.07010
712	12	7.2957549	1861.9448	124.05050
713	13	7.2683396	1895.4423	120.66061

Antoine Constants

Series Name: Acids

Pressure Range (mm Hg) - Top: .99 E 49

Bottom: .99 E-49

Series Code: 700

Compound Code	Carbon Number	Antoine Constants A	B	C
714	14	-	-	-
715	15	7.0242660	1811.8718	99.783514
716	16	7.0862038	1866.8956	95.995755
717	17	7.2029265	1978.4443	99.258815
718	18	7.1168953	1959.1987	91.568691

Antoine Constants

Series Name: Acids

Pressure Range (mm Hg) - Top: 10,000
Bottom: 30

Series Code: 700

Compound Code	Carbon Number	Antoine Constants A	B	C
701	1	-	-	-
702	2	7.4621617	1580.1156	226.73193
703	3	6.5990600	1080.4775	148.83693
704	4	-	-	-
705	5	-	-	-
706	6	6.6654014	1204.6694	112.48309
707	7	7.5521603	1802.5491	162.88965
708	8	6.6927352	1292.0990	99.711986
709	9	7.3274102	1742.4221	136.83272
710	10	6.9877481	1560.9470	110.05798
711	11	6.9992467	1612.9498	107.48717
712	12	6.5055266	1337.4260	70.020035
713	13	6.6253946	1455.2409	76.259863

Antoine Constants

Series Name: Acids

Pressure Range (mm Hg) - Top: 10,000

Bottom: 30

Series Code: 700

Compound Code	Carbon Number	Antoine Constants A	B	C
714	14	-	-	-
715	15	6.2519491	1303.2144	46.521497
716	16	6.1743828	1270.1428	33.633020
717	17	5.6663945	996.68366	-8.3901574
718	18	-	-	-

Antoine Constants

Series Name: Acids

Pressure Range (mm Hg) - Top: 30

Bottom: .99 E-49

Series Code: 700

Compound Code	Carbon Number	Antoine Constants A	B	C
701	1	-	-	-
702	2	6.3691090	1130.1480	1932.3421
703	3	0.86097796	-4.3065170	-28.161167
704	4	-	-	-
705	5	-	-	-
706	6	9.1577704	2751.2343	238.73164
707	7	8.9972289	2690.0745	224.07857
708	8	7.8134046	2018.3988	170.80377
709	9	7.9896323	2192.5298	175.53684
710	10	7.5982746	1980.9356	150.39868
711	11	8.2761125	2479.3336	179.77934
712	12	7.6437359	2052.8604	137.31854
713	13	7.8375444	2272.1358	150.07831

Antoine Constants

Series Name: Acids

Pressure Range (mm Hg) - Top: 30

Bottom: .99 E-49

Series Code: 700

Compound Code	Carbon Number	Antoine Constants A	B	C
714	14	-	-	-
715	15	8.1556754	2554.5491	155.44862
716	16	7.3344433	2023.7383	108.56714
717	17	8.4092306	2790.3863	156.66095
718	18	-	-	-

Antoine Constants

Series Name: Acids

Pressure Range (mm Hg) - Top: 10,000 50,000

Bottom: 1 760

Series Code: 700

Compound Code		Carbon Number	Antoine Constants A	B	C
702	50,000 760	2	8.0332624	2037.9857	277.82508
712	10,000 1	12	7.1355092	1757.9811	114.97314
714	10,000 1	14	7.1572742	1857.1055	109.67433

Antoine Constants

Series Name: Esters-Formate

Pressure Range (mm Hg) - Top: Bottom: (Mixed)

Series Code: 800

Compound Code	Carbon Number	Antoine Constants A	B	C
Methyl Formate				
801 40,000 0	2	7.2137593	1150.4237	233.62275
801 40,000 760	2	7.1802054	1132.4727	231.63739
801 10,000 30	2	7.2235608	1155.0755	234.09831
Ethyl Formate				
802 40,000 0	3	7.1232822	1189.0837	225.93155
802 40,000 760	3	7.2782332	1310.3340	244.04846
802 10,000 30	3	7.1364140	1193.9770	226.26731
802 30 0	3	0.79003075	12.356041	-2.2777777

Antoine Constants

Series Name: Esters-Formate

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 800

Compound Code	Carbon Number	Antoine Constants A	B	C
n-Propyl Formate				
803 .99 E 49 .99 E-49	4	7.1244009	1287.4009	222.21992
803 40,000 760	4	7.1365604	1314.0790	227.84321
803 10,000 30	4	7.0602211	1249.5711	217.94057
803 30 0	4	2.4206999	69.517731	61.096363
n-Butyl Formate				
804 .99 E 49 .99 E-49	5	7.1452822	1368.6046	215.20744

Antoine Constants

Series Name: Esters-Acetate

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 900

Compound Code	Carbon Number	Antoine Constants A	B	C
Methyl Acetate				
901 .99 E 49 .99 E-49	3	7.2679741	1267.7990	231.62706
901 40,000 760	3	7.3422055	1328.7872	240.68202
901 10,000 35	3	7.0766506	1159.8672	219.26346
901 35 0	3	2.9229648	85.107860	71.625551
Ethyl Acetate				
902 .99 E 49 .99 E-49	4	7.1638075	1277.2488	220.99080
902 40,000 760	4	7.3127172	1393.8571	237.44104
902 10,000 30	4	7.102881	1244.0414	217.45508
902 30 0	4	0.79947966	0.046197	17.230351

Antoine Constants

Series Name: Esters-Acetate

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 900

Compound Code	Carbon Number	Antoine Constants A	B	C
Propyl Acetate				
903 .99 E 49 .99 E-49	5	7.0719056	1314.2710	211.75953
903 10,000 30	5	7.1014966	1323.9272	212.06702
903 30 0	5	5.5495117	745.75557	159.52177

Antoine Constants

Series Name: Esters-Propionate

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 1000

Compound Code	Carbon Number	Antoine Constants A	B	C
Methyl n-Propionate				
1001 .99 E 49 .99 E-49	4	7.0990194	1253.6299	217.49561
1001 40,000 760	4	7.3703685	1452.9046	244.00517
1001 10,000 30	4	7.128754	1272.0894	219.63888
1001 30 0	4	2.012580	41.033498	52.470854
Ethyl Propionate				
1002 .99 E 49 .99 E-49	5	7.0882397	1309.0949	211.97070
1002 40,000 760	5	7.3868628	1547.7952	244.44870
1002 10,000 30	5	7.0298900	1278.8818	209.00208
1002 30 0	5	7.0478195	1294.7227	211.02059
Propyl Propionate				
1003 .99 E 49 .99 E-49	6	7.0708880	1391.2516	208.88206

Antoine Constants

Series Name: Esters-Butyrate

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 1100

Compound Code	Carbon Number	Antoine Constants A	B	C
Methyl n-Butyrate				
1101 1,000 1.0	5	4.1891877	222.06595	57.600813
Ethyl Butyrate				
1102 .99 E 49 .99 E-49	6	6.8923254	1315.8758	206.19269
1102 10,000 30	6	5.2353962	529.88304	101.72692

Antoine Constants

Series Name: Esters-Caproate

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 1300

Compound Code	Carbon Number	Antoine Constants A	B	C
Methyl Caproate				
1301 .99 E 49 .99 E-49	7	7.3826374	1654.7428	217.26164
1301 10,000 30	7	7.4496703	1698.1295	221.43313
1301 30 0	7	-1.9428087	479.68267	-202.94517

Antoine Constants

Series Name: Esters-Caprylate

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 1500

Compound Code	Carbon Number	Antoine Constants A	B	C
Methyl Caprylate				
1501 .99 E 49 .99 E-49	9	7.6063329	1921.9957	214.8351
1501 10,000 30	9	6.3122596	1154.1629	139.79120
1501 30 0	9	6.8868476	1552.1372	187.52390

Antoine Constants

Series Name: n-Alkyl Benzene

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 1800

Compound Code	Carbon Number	Antoine Constants A	B	C
Toluene				
1801 40,000 1	7	7.0633796	1405.5455	225.57706
1801 40,000 760	7	6.9695755	1325.4017	213.52047
1801 10,000 30	7	7.129401	1448.0809	230.32819
1801 30 0	7	6.2258374	1051.3484	195.06069
Ethyl Benzene				
1802 .99 E 49 .99 E-49	8	7.0223067	1461.9570	216.98351
1802 10,000 30	8	6.7811594	1313.9248	200.73693
1802 30 0	8	6.3582200	1166.9825	191.99411

Antoine Constants

Series Name: n-Alkyl Benzene

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 1800

Compound Code	Carbon Number	Antoine Constants A	B	C
Propyl Benzene				
1803 .99 E 49 .99 E-49	9	6.1659255	1020.4348	151.00346
n-Butyl Benzene				
1804 .99 E 49 .99 E-49	10	7.1253272	1677.5158	212.00318
1810 .99 E 49 .99 E-49	16	7.0496075	1915.3968	161.56918
1812 .99 E 49 .99 E-49	18	7.9761096	2648.1424	231.11992

Antoine Constants

Series Name: n-Mono Olefins

Pressure Range (mm Hg) - Top: .99 E 49

Bottom: .99 E-49

Series Code: 1900

Compound Code	Carbon Number	Antoine Constants A	B	C
1901	BP = 101.2°C @ 760 mm	6.4431113	1062.0955	197.01043
1902	BP = 131.7°C @ 760 mm	6.8802605	1390.0065	215.77658
1903	BP = 156.5°C @ 76 mm	6.8967946	1467.0019	208.57420
1904	BP = 181°C @ 760 mm	6.9232499	1546.8018	201.69428

Antoine Constants

Series Name: n-Alkyl Cyclo Hexane

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 2000

Compound Code	Carbon Number	Antoine Constants A	B	C
Ethyl Cyclo Hexane				
2002	40,000 1	6.6752900	537.43650	246.10714
2002	40,000 760	7.4595500	908.44450	306.07000
2002	10,000 30	6.8753474	608.66030	256.62852
2002	30 0	-2.9532953	44.833030	143.34708
2003	40,000 1	6.9505456	836.11564	252.90755
2003	40,000 760	6.9386640	827.48877	251.11583
2003	10,000 30	6.9862834	857.94413	256.41987
2003	30 0	8.0148493	1110.3138	270.57564

Antoine Constants

Series Name: n-Alkyl Cyclo Hexane

Pressure Range - Top: (mm Hg) Bottom: (Mixed)

Series Code: 2000

Compound Code	Carbon Number	Antoine Constants A	B	C
2004 40,000 1		6.7970260	904.34650	237.30161
2004 40,000 760		7.1912392	1131.2743	269.46937
2004 10,000 30		6.9244190	968.79971	245.86782
2004 30 0		8.5425225	1445.1306	272.40731
2005 10,000 30		7.9843520	1731.7164	309.22004
2005 30 0		8.6588163	2092.5532	334.31747
2006		6.7040775	1071.4459	216.62552
2007		6.4204023	1029.7234	196.52488
2008		6.8835433	1326.4689	210.00136
2009		6.9770156	1450.1395	207.15718
2010		6.9519845	1498.7581	197.46998
2012		6.2930143	1170.1372	129.22445

Antoine Constants

Series Name: n-Alkyl Cyclo Hexane

Pressure Range (mm Hg) - Top: Bottom: (Mixed)

Series Code: 2000

Compound Code	Carbon Number	Antoine Constants A	B	C
2015		7.0149494	1781.7191	162.57852
2016		7.0992069	1892.2551	163.42170

Antoine Constants

Series Name: n-Paraffins

Pressure Range (mm Hg) - Top: 40,000

Bottom: 1

Series Code: 2100

Compound Code	Carbon Number	Antoine Constants A	B	C
2101	1	-	-	-
2102	2	7.0082951	728.99790	264.49172
2103	3	7.0386907	905.86205	260.13187
2104	4	6.8702482	962.98214	242.26056
2105	5	6.9429470	1109.1189	236.95661
2106 70,000 1	6	6.8053387	1138.8075	221.12650
2107	7	6.7542111	1184.2502	207.42521
2108	8	7.0157284	1406.7522	214.59077
2109	9	-	-	-
2110	10	6.9717700	1512.8543	195.70911
2111	11	-	-	-
2112	12	6.8859308	1576.8284	177.24106
2113	13	-	-	-
2114	14	-	-	-
2115	15	-	-	-
2116	16	-	-	-

Antoine Constants

Series Name: n-Paraffins

Pressure Range (mm Hg) - Top: 40,000
Bottom: 760

Series Code: 2100

Compound Code	Carbon Number	Antoine Constants A	B	C
2101	1	7.1213140	526.20790	286.03057
2102	2	7.1607650	803.24220	276.49688
2103	3	7.0366109	900.70136	258.67153
2104	4	7.0137080	1020.9319	247.29226
2105	5	7.1682711	1262.5803	258.43259
2106 70,000 760	6	6.2158664	730.37114	149.91298
2107	7	7.2716556	1542.8531	252.94426
2108	8	7.4244717	1766.4468	263.55755
2109	9	-	-	-
2110	10	-	-	-
2111	11	-	-	-
2112	12	6.8170876	1466.9391	156.51534
2113	13	-	-	-
2114	14	-	-	-
2115	15	-	-	-
2116	16	-	-	-

Antoine Constants

Series Name: n-Paraffins

Pressure Range (mm Hg) - Top: 10,000
Bottom: 30

Series Code: 2100

Compound Code	Carbon Number	Antoine Constants A	B	C
2101	1	6.6145440	386.31430	265.03493
2102	2	6.9298430	702.41480	262.08073
2103	3	7.1122893	947.35170	266.19404
2104	4	6.9166595	991.86722	246.57916
2105	5	6.8407560	1060.6086	231.70190
2106	6	6.9294518	1201.1231	227.73492
2107	7	6.9432279	1293.1676	219.83287
2108	8	6.8923549	1330.7252	206.15781
2109	9	-	-	-
2110	10	-	-	-
2111	11	-	-	-
2112	12	6.9130225	1567.8229	173.19644
2113	13	-	-	-
2114	14	-	-	-
2115	15	-	-	-
2116	16	6.8976623	1729.2282	143.55947

Antoine Constants

Series Name: n-Paraffins

Pressure Range (mm Hg) - Top: 30
Bottom: 0

Series Code: 2100

Compound Code	Carbon Number	Antoine Constants A	B	C
2101	1	7.4218438	493.44090	272.36968
2102	2	6.8297384	671.65790	258.02609
2103	3	6.4636544	727.21262	243.11772
2104	4	6.7640037	927.22884	238.94187
2105	5	7.3248083	1219.0446	242.81574
2106	6	4.4152178	377.55898	135.55052
2107	7	3.8296260	294.02071	107.46449
2108	8	6.2101454	1055.4241	183.35529
2109	9	-	-	-
2110	10	-	-	-
2111	11	-	-	-
2112	12	3.4917289	364.47215	57.155442
2113	13	-	-	-
2114	14	-	-	-
2115	15	-	-	-
2116	16	6.0604684	1439.0598	136.16741

Antoine Constants

Series Name: n-Paraffins

Pressure Range (mm Hg) - Top: .99 E 49

Bottom: .99 E-49

Series Code: 2100

Compound Code	Carbon Number	Antoine Constants A	B	C
2109	9	6.9536487	1440.3454	202.86477
2111*	11	.46439060	230.91821	284.67488
2115	15	6.7532910	1600.0919	142.26851

*Poor

Antoine Constants

Series Name:

Pressure Range (mm Hg) - Top:
Bottom: (Mixed)

Series Code: 2200

Compound Code	Carbon Number	Antoine Constants A	B	C
2201 .99 E 49 .99 E-49		7.3291082	1876.2962	189.95490
2201 10,000 30		6.9575326	1625.4578	165.78423
2201 30 0		7.3696994	1898.6810	191.57727

Antoine Constants

Series Name:

Pressure Range (mm Hg) - Top:
Bottom:
(Mixed)

Series Code: 2300

Compound Code	Carbon Number	Antoine Constants A	B	C
2301 .99 E 49 .99 E-49		7.3466910	1984.8289	178.15338
2301 10,000 30		6.6982014	1544.7482	135.78168
2301 30 0		7.3124798	1967.1370	177.00323

Antoine Constants

Series Name:

Pressure Range (mm Hg) - Top: (Mixed)
Bottom:

Series Code: 2600

Compound Code	Carbon Number	Antoine Constants A	B	C
2601 .99 E 49 .99 E-49		6.9854358	1861.8688	151.91728
2601 10,000 30		4.2168884	372.20182	-52.765863
2601 30 0		6.2541242	1476.7160	121.75234

APPENDIX D

Internal Heat of Vaporization

Series Name: Alcohols

Series Code: 100

Kemme-Kreps Constants for Effective Chain Length Power, PW

A = 0.73507×10^4
B = 0.22142×10^3
C = 0.23166×10^4

PW = 0.666

Correlation Coefficient: 0.97389

Variance of Estimate: 0.294192×10^6

Carbon Number, N	$N^{(PW)}$	Calculated Internal Heat of Vaporization @ 5 mmHg	50 mmHg	200 mmHg	760 mmHg
1	1.00	9311.0	8801.2	8494.2	8198.6
2	1.59	10461.0	9652.1	9165.1	8696.0
5	2.92	13076.5	11587.3	10690.7	9827.3
6	3.30	13815.7	12134.3	11121.9	10147.1
7	3.66	14514.7	12651.4	11529.7	10449.4
8	4.00	15181.0	13144.4	11918.4	10737.6
10	4.64	16435.6	14072.7	12650.2	11280.3
12	5.24	17608.5	14940.6	13334.4	11787.6

Internal Heat of Vaporization

Series Name: Alcohols

Series Code: 100

Kemme-Kreps Constants for Effective Chain Length Power, PW

$A = 0.75850 \times 10^4$
$B = 0.24384 \times 10^3$
$C = 0.23816 \times 10^4$

PW = 0.666

Correlation Coefficient: 0.99040

Variance of Estimate: 0.104681×10^6

Carbon Number, N	$N^{(PW)}$	Calculated Internal Heat of Vaporization @ 5 mmHg	50 mmHg	200 mmHg	760 mmHg
1	1.00	9574.1	9012.7	8674.6	8349.1
2	1.59	10741.1	9850.2	9313.9	8797.4
3	2.08	11719.5	10552.5	9849.9	9173.3
4	2.52	12592.6	11179.2	10328.2	9508.7
6	3.30	14145.1	12293.4	11178.6	10105.0
7	3.66	14854.3	12802.5	11567.1	10377.5
8	4.00	15530.4	13287.7	11937.5	10637.2
10	4.64	16803.5	14201.5	12634.9	11126.3
12	5.24	17993.7	15055.7	13286.8	11583.5

Internal Heat of Vaporization

Series Name: Alkyl Hallides (CL)

Series Code: 400

Kemme-Kreps Constants for Effective Chain Length Power, PW

$A = 0.37591 \times 10^4$
$B = 0.13327 \times 10^3$
$C = 0.20122 \times 10^4$

PW = 0.666

Correlation Coefficient: 0.98623

Variance of Estimate: 0.441498×10^5

Carbon Number, N	$N^{(PW)}$	Calculated Internal Heat of Vaporization @ 5 mmHg	50 mmHg	200 mmHg	760 mmHg
1	1.00	5556.9	5250.0	5065.3	4887.3
2	1.59	6611.6	6124.7	5831.5	5549.2
4	2.52	8285.0	7512.4	7047.3	6599.4
5	2.92	9010.1	8113.8	7574.2	7054.5

Internal Heat of Vaporization

Series Name: Acids

Series Code: 700

Kemme-Kreps Constants for Effective Chain Length Power, PW

$A = 0.70369 \times 10^4$
$B = 0.18949 \times 10^3$
$C = 0.25485 \times 10^4$

PW = 0.666

Correlation Coefficient: 0.98726

Variance of Estimate: 0.301449×10^6

Carbon Number, N	$N^{(PW)}$	Calculated Internal Heat of Vaporization @ 5 mmHg	50 mmHg	200 mmHg	760 mmHg
1	1.00	9280.4	8844.1	8581.4	8328.4
2	1.59	10596.6	9904.3	9487.5	9086.1
6	3.30	14435.9	12997.0	12130.6	11296.4
7	3.66	15235.9	13641.4	12681.4	11756.9
8	4.00	15998.5	14255.6	13206.3	12195.9
9	4.33	16729.8	14844.7	13709.8	12616.9
10	4.64	17434.3	15412.2	14194.8	13022.5
11	4.96	18115.7	15961.1	14663.9	13414.7
12	5.24	18776.7	16493.6	15118.9	13795.2
13	5.52	19419.5	17011.4	15561.5	14165.3
15	6.07	20657.7	18008.7	16413.9	14878.1
16	6.33	21255.9	18490.6	16825.8	15223.5
17	6.60	21841.7	18962.5	17229.1	15559.7
18	6.85	22416.2	19425.3	17624.5	15890.4

Internal Heat of Vaporization

Series Name: Acids

Series Code: 700

Kemme-Kreps Constants for Effective Chain Length Power, PW

$A = 0.74295 \times 10^4$
$B = 0.29473 \times 10^3$
$C = 0.29764 \times 10^4$

PW = 0.666

Correlation Coefficient: 0.98301

Variance of Estimate: 0.425580×10^6

Carbon Number, N	$N^{(PW)}$	Calculated Internal Heat of Vaporization @ 5 mmHg	50 mmHg	200 mmHg	760 mmHg
2	1.59	11399.5	10322.7	9674.4	9050.1
3	2.08	12630.2	11219.6	10370.3	9552.5
6	3.30	15681.3	13443.2	12095.6	10798.0
7	3.66	16573.5	14093.3	12600.1	11162.2
8	4.00	17423.9	14713.1	13081.0	11509.4
9	4.33	18239.5	15307.5	13542.2	11842.3
10	4.64	19025.3	15880.1	13986.6	12163.1
11	4.96	19785.2	16434.0	14416.3	12473.3
12	5.24	20522.4	16971.2	14833.1	12774.2
13	5.52	21239.3	17493.6	15238.5	13066.8
15	6.07	22620.2	18499.9	16019.4	13630.5
16	6.33	23287.4	18986.2	16396.6	13902.9
17	6.60	23940.8	19462.4	16766.1	14169.6

Internal Heat of Vaporization

Series Name: Esters-Formate

Series Code: 800

Kemme-Kreps Constants for Effective Chain Length Power, PW

$A = 0.45560 \times 10^4$
$B = 0.14667 \times 10^3$
$C = 0.19860 \times 10^4$

PW = 0.666

Correlation Coefficient: 0.99293

Variance of Estimate: 0.120290×10^5

Carbon Number, N	$N^{(PW)}$	Calculated Internal Heat of Vaporization @ 5 mmHg	50 mmHg	200 mmHg	760 mmHg
2	1.59	7332.6	6796.8	6474.1	6163.5
3	2.08	8193.4	7491.4	7068.8	6661.8
4	2.52	8961.6	8111.4	7599.5	7106.5
5	2.92	9667.5	8681.0	8087.1	7515.2

Internal Heat of Vaporization

Series Name: n-Alkyl Benzene

Series Code: 1800

Kemme-Kreps Constants for Effective Chain Length Power, PW

$A = 0.20055 \times 10^4$

$B = 0.10101 \times 10^3$

$C = 0.21761 \times 10^4$

$PW = 0.666$

Correlation Coefficient: 0.97033

Variance of Estimate: 0.338904×10^6

Carbon Number, N	$N^{(PW)}$	Calculated Internal Heat of Vaporization @ 5 mmHg	50 mmHg	200 mmHg	760 mmHg
7	3.66	9363.9	8513.9	8002.2	7509.4
8	4.00	10048.4	9119.3	8559.9	8021.3
9	4.33	10704.7	9699.8	9094.8	8512.2
10	4.64	11337.0	10259.1	9610.2	8985.2
16	6.33	14766.9	13292.8	12405.3	11550.1
18	6.85	15808.2	14213.8	13253.9	12329.5

Internal Heat of Vaporization

Series Name: n-Akyl Benzene

Series Code: 1800

Kemme-Kreps Constants for Effective Chain Length Power, PW

$A = 0.75549 \times 10^3$
$B = 0.10668 \times 10^3$
$C = 0.25130 \times 10^4$

PW = 0.666

Correlation Coefficient: 0.98373

Variance of Estimate: 0.166536×10^3

Carbon Number, N	$N^{(PW)}$	Calculated Internal Heat of Vaporization @ 200 mmHg	760 mmHg	5000 mmHg	10,000 mmHg
7	3.66	7873.8	7353.3	6618.9	6348.6
8	4.00	8535.9	7967.0	7164.2	6868.8
9	4.33	9170.8	8555.5	7687.2	7367.7
10	4.64	9782.5	9122.4	8191.0	7848.4
16	6.33	13100.4	12197.7	10924.0	10455.3
18	6.85	14107.7	13131.4	11753.8	11246.9

Internal Heat of Vaporization

Series Name: n-Mono Olefins

Series Code: 1900

Kemme-Kreps Constants for Effective Chain Length Power, PW

$A = -0.27817 \times 10^3$
$B = 0.12240 \times 10^3$
$C = 0.27289 \times 10^4$

PW = 0.666

Correlation Coefficient: 0.99909

Variance of Estimate: 0.246391×10^5

Carbon Number, N	$N^{(PW)}$	Calculated Internal Heat of Vaporization @ 5 mmHg	50 mmHg	200 mmHg	760 mmHg
2	1.59	3740.7	3293.3	3023.9	2764.6
3	2.08	4987.9	4401.7	4048.8	3708.9
4	2.52	6101.1	5391.0	4963.4	4551.7
5	2.92	7124.3	6300.2	5804.1	5326.3
6	3.30	8080.9	7150.3	6590.1	6050.6
7	3.66	8985.5	7954.3	7333.4	6735.5
8	4.00	9847.9	8720.6	8041.9	7388.4
9	4.33	10675.0	9455.7	8721.6	8014.6
10	4.64	11471.9	10163.9	9376.4	8618.0
11	4.96	12242.6	10848.8	10009.7	9201.6
12	5.24	12990.4	11513.3	10624.0	9767.6
13	5.52	13717.5	12159.5	11221.5	10318.2
14	5.81	14426.3	12789.4	11803.9	10854.8
15	6.07	15118.4	13404.4	12372.5	11378.8
16	6.63	15795.2	14005.9	12928.7	11891.3
17	6.60	16458.1	14595.0	13473.3	12393.1
18	6.85	17108.0	15172.6	14007.4	12885.2

Internal Heat of Vaporization

Series Name: n-Paraffins

Series Code: 2100

Kemme-Kreps Constants for Effective Chain Length Power, PW

A = 0.30684×10^2
B = 0.12104×10^3
C = 0.27013×10^4

PW = 0.666

Correlation Coefficient: 0.9995872

Variance of Estimate: 0.110182×10^5

Carbon Number, N	$N^{(PW)}$	Calculated Internal Heat of Vaporization @ 5 mmHg	50 mmHg	200 mmHg	760 mmHg
2	1.59	3948.0	3505.6	3239.2	2982.7
3	2.08	5182.7	4603.0	4254.0	3917.9
4	2.52	6284.8	5582.5	5159.7	4752.6
5	2.92	7297.6	6482.8	5992.2	5519.7
6	3.30	8244.7	7324.5	6770.5	6237.0
7	3.66	9140.3	8120.5	7506.5	6915.3
8	4.00	9994.0	8879.3	8208.2	7561.9
9	4.33	10812.8	9607.1	8881.2	8182.1
10	4.64	11601.8	10308.3	9529.6	8779.6
11	4.96	12364.8	10986.5	10156.7	9357.5
12	5.24	13105.1	11644.4	10765.0	9918.2
13	5.52	13825.0	12284.3	11356.7	10463.4
14	5.81	14526.6	12907.9	11933.4	10994.9
15	6.07	15211.8	13516.9	12496.4	11513.8
16	6.33	15881.8	14112.4	13047.2	12021.3
17	6.60	16538.1	14695.7	13586.5	12518.3
18	6.85	17181.5	15267.6	14115.3	13005.7

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