Molecular Structure and Physical Properties of Branched Alkanes

Koichiro NAKANISHI*

(Received June 15, 1961)

The isomeric variation in the physical properties of branched alkanes (isoparaffins) is an interesting problem in the field of the study on the correlation between the molecular structure and the physical properties of organic compounds. Owing to the absence of polarity (dipole moment is nearly equal to zero), the properties of paraffin hydrocarbons depend only on the shape of molecule, namely, on the number of carbon atoms in the molecule and on the number and relative position of the side chains. A number of investigations have been made to clarify this dependence.[1-18] Of these, a method proposed by Wiener[8] is the most favorable. In spite of its simplicity, Wiener's parameters are able to predict the structural variation in isoparaffins with sufficient accuracy. We have also adopted this set of parameters to correlate the "effective carbon number" with the molecular structure of the isoparaffins in our previous paper[19] (this paper will be referred to as P-I).

Detailed examination, however, reveals that some systematic deviations of estimated value from the experimental are observed in the case of the definite types of compounds whenever we use the Wiener parameters. Greenshields and Rossini[20] have recently obtained an improved correlation with additional terms by which such deviations are to be eliminated. Although this improvement is effective for the purpose of more accurate prediction of many physical properties, physical meaning of the additional parameters is not clear.

In the course of the study on the structural variation in alkenes,[21] we have arrived at a new correlation expressing the difference of "effective carbon number" of alkenes from the real carbon number in terms of new structural parameters. This correlation contains an expression for branched alkanes as a special case and will be also effective to predict the isomeric variation in isoparaffins. The purpose of this paper is to present a comparison

*Assistant Professor of Industrial Chemistry, Faculty of Engineering, Shinshu University, Nagano, Japan.

of the estimated values by the proposed equation with experimental data in great details and to discuss the results in terms of the physical meaning of effective carbon number and the structural parameters.

Definition and Experimental Proof of Effective Carbon Number

Let us first define the "effective carbon number" of isoparaffins. When the boiling points of normal paraffins are plotted against the number of carbon atoms, a family of curves for different pressures is obtained. Then, reading the boiling points of a given isoparaffin on these curves, we can obtain a set of values of an effective number of carbon atoms, each corresponding to every different pressure. If this effective number does not dependent on the external conditions, i. e., independent of pressure, it is treated as a structural constant depending only on the strucutural feature of each compound.

From an extensive experimental test shown in Table I and Figure 1, we can conclude that a reasonable constancy of the values is observed over a wide range of pressure and that these numbers can be regarded, as a first approximation, as characteristic constants. We will call this number as the "effective carbon number" and hereafter denoted by n^*.

It can be shown later that the proper assignment of the n^* value is advantageous not only to the estimation of the vapor pressure curve of isoparaffins but also to that of other physical properties such as critical constants. Thus, replacing the real carbon number n by n^*, the following equations which have been derived in P-I can be applied to isoparaffins (and also for linear and branched olefins).

$$T_b{}^o = \frac{127.55\, n^{*2/3}}{1 + 0.070\,33\, n^{*2/3}}, \tag{1}$$

$$n^{*2/3}/T_b = [0.007\,840 - 0.002\,15 \log P - 0.000\,10 (\log P)^2] + (0.000\,551\,4 - 0.000\,011 \log P) n^{*2/3}, \tag{2}$$

$$A = \frac{2\,128\, n^{*2/3}}{1 + 0.005\,12\, n^{*2/3} + 0.093\,0 \log P}, \tag{3}$$

$$A^o = 2\,146\, n^{*2/3} \left[\frac{1 + 0.062\,02\, n^{*2/3}}{1 + 0.070\,33\, n^{*2/3}}^3\right], \tag{4}$$

$$\frac{1}{T_c} = 0.000\,702 + \frac{0.004\,192}{n^{*2/3}}, \tag{5}$$

$$P_c = \frac{80.37}{n^{*2/3}(1 + 0.1675\, n^{*2/3})}, \tag{6}$$

$$V_c = 0.0412\,(n^{*2/3} + n^*). \tag{7}$$

where T_b^o is normal boiling point in ^oK, T_b is boiling point in ^oK, P is pressure in atmosphere, Δ is heat of vaporization in cal/mol, Δ^o is heat of vaporization at normal boiling point in cal/mol, T_c is the critical temperature in ^oK, P_c is the critical pressure in atmosphere and V_c is the critical volume in cc/mol.

However, calculation by equations (1) to (7) is quite troublesome since n^* is, in general, not integral. Graphical method is preferable for this reason. The nomograms presented in P–I will be quite useful for this purpose.

Structural Units

Once definition of effective carbon number n^* is established, the next step is to find an equation which correlates the effective carbon number with the structural formula of compound. One of the excellent ways is to adopt the Wiener parameters as in P–I. But the Wiener parameters are not applicable to the structural specification of olefinic hydrocarbons. On the contrary, our new structural parameters proposed in our recent paper[21] (this paper will be referred to as P–II) can describe the structural feature of both isoparaffins and olefins. For the reasons given above and also in later section, we will adopt here the latter parameters. We shall now explain our method briefly.

The molecular structures of isoparaffins can be specified by the number and the relative position of the two kinds of branching units, i. e., tertiary and quaternary carbon atoms. If the mutual influence among them is properly factorized, the deviation of the effective carbon number from the real one may be expressed by a linear combination of two factors, each corresponding to branching units. Although various kinds of methods for such factorization would be possible, only the linear factorization is used because of its simplicity for practical purposes.

The contribution of two structural units, trifunctional branching (I) and tetrafunctional branching (II)

(I) $-C-\underset{\displaystyle C}{\overset{\displaystyle |}{C}}-C-$ (II) $-C-\underset{\displaystyle C}{\overset{\displaystyle C}{\overset{\displaystyle |}{\underset{\displaystyle |}{C}}}}-C-$

to the effective carbon number of compound is expressed by the following equations, which are obtained after some troublesome analysis of available boiling point data:[21~23]

$$\Delta n_I = 0.28 - 0.06c_2 + 0.06c_3, \tag{8}$$

$$\Delta n_{II} = 0.73 - 0.14c_2 + 0.05c_3. \tag{9}$$

The difference between the effective carbon number n^* and the real carbon number n is then given by the sum of these two contributions,

$$\Delta n = n - n^* = \Sigma_I \Delta n_I + \Sigma_{II} \Delta n_{II}, \tag{10}$$

where the summation extends over all structural units of each type. The two parameters, c_2 and c_3, in equations (8) and (9) are defined as follows:

c_2 —— the number of the second neighbor carbon atoms of the branching point (tertiary or quaternary carbon atom).

c_3 —— the number of the third neighbor carbon atoms of the branching point (tertiary or quaternary carbon atom).

Illustration : Examples of Calculation

We will now summarize our method recommended for the prediction of some physical properties of isoparaffins.

Recommended Method

(1) The effective carbon number n^* is first calculated by equation (10). Only the structural formula of isoparaffin in question is required.

(2) The vapor pressure-temperature relationship, critical temperature, critical pressure and the heat of vaporization at normal boiling point can be read on nomogram[19] by using the value of n^* obtained in (1).

(3) The heat of vaporization as a function of temperature can be calculated by substituting the value of n^* obtained in the procedure (1) into equation (3). However the use of Watson's equation is preferable in this case,

$$\log \Delta = \log \Delta^o + 0.38 \log \frac{T_c - T}{T_c - T_b{}^o}, \tag{11}$$

where the values of Δ^o, T_c and $T_b{}^o$ are obtained from the procedures (1) and (2).

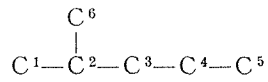
(4) The critical volume is calculated by equation (7).

(5) If one boiling point datum is available, the procedure (1) becomes

unnecessary. By the reverse procedure of (2), n^* will be determined graphically on nomogram.

For the clear understanding of the recommended method, we will present some examples of calculation.

A) 2-Methylpentane



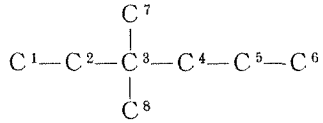
This compound contains one tertiary carbon atom C^2. It has one second neighbor, say C^4, and one third neighbor, say C^5, respectively, hence

$$\Delta n = \Delta n = 0.28 - 0.06 \times 1 + 0.06 \times 1 = 0.28,$$

$$n^* = n - \Delta n = 6 - 0.28 = 5.72.$$

Then, using the nomogram, 60°C is obtained for the normal boiling point which is to be compared with the observed value of 60.3°C.[22] For the critical pressure and temperature, 30 atm. and 497°K are obtained, while the experimental data are 30 atm. and 498.1°K.[22] The heat of vaporization at normal boiling point can be also read on nomogram as 6.70 Kcal/mol. This value is to be compared with the literature value of 6.626 Kcal/mol.[22] Substituting $A^o = 6.70$, $T_c = 497$, $T_b^o = 333$ and $T = 298$ (25°C) into equation (11), the standard heat of vaporization is calculated as 7.20 Kcal/mol, which is to be compared with the literature value of 7.183 Kcal/mol.[22] The agreement of calculated values with experimental data is highly satisfactory.

B) 3,3-Dimethylhexane



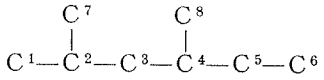
This compound has one quaternary carbon atom C^3. It has two second neighbors, say C^1 and C^5, and one third neighbor C^6. Then,

$$\Delta n = \Delta n_{11} = 0.73 - 0.14 \times 2 + 0.05 \times 1 = 0.50,$$

$$n^* = n - \Delta n = 8 - 0.50 = 7.50.$$

The value of n^* at normal boiling point is estimated to be 7.51.

C) 2,4-Dimethylhexane



There are two tertiary carbon atoms C^2 and C^4 in this molecule. The contributions of these two to Δn are calculated separately.

Tertiary carbon atom C^2: second neighbor $= C^4$ $c_2 = 1$

third neighbor $= C^5$ and C^8 $c_3 = 2$

$$\Delta n(C^2) = 0.28 - 0.06 \times 1 + 0.06 \times 2 = 0.34.$$

Tertiary carbon atom C^4: second neighbor $= C^2$ and C^6 $c_2 = 2$

third neighbor $= C^1$ and C^7 $c_3 = 2$

$$\Delta n(C^4) = 0.28 - 0.06 \times 2 + 0.06 \times 2 = 0.28;$$

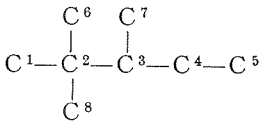
then,

$$\Delta n = \Delta n\,(C^2) + \Delta n\,(C^4) = 0.34 + 0.28 = 0.62,$$

$$\therefore \quad n^* = n - \Delta n = 8 - 0.62 = 7.38;$$

n^* at normal boiling point being 7.41.

D) 2, 2, 3-Trimethylpentane



This molecule has one tertiary carbon atom C^3 and one quaternary carbon atom C^2.

Tertiary carbon atom C^3:

second neighbor $= C^1$, C^5, C^6 and C^8 $c_2 = 4$,

third neighbor $=$ None $c_3 = 0$,

$$\Delta n\ (C^3) = 0.28 - 0.06 \times 4 = 0.04.$$

Quaternary carbon atom C^2:

second neighbor $= C^4$ and C^7 $c_2 = 2$,

third neighbor $= C^5$ $c_3 = 1$.

$$\Delta n_{II}(C^2) = 0.73 - 0.14 \times 2 + 0.05 \times 1 = 0.50.$$

Then, Δn is given as the sum of the above two.

$$\Delta n = \Delta n_I + \Delta n_{II} = 0.04 + 0.50 = 0.54,$$

$$n^* = n - \Delta n = 8 - 0.54 = 7.46.$$

While n^* at $T_b{}^o$ is estimated to be 7.43.

Comparison with Experimental Data

Experimental data of boiling point and other physical properties of isoparaffins have been collected extensively in monographs or reviews by Egloff,[23] Stull,[24] Ferris[25] and others. The most extensive and systematic work was done by Rossini and his colleagues[22] who published a selected value of physical properties of hydrocarbons and related compounds.

We will now test the utility of the recommended method by comparing the predicted value with these literature values. This test is made with 117 isoparaffins ranging from C_4H_{10} (isomers of *n*–Butane) to $C_{11}H_{24}$ (isomers of n–Undecane). Table II shows the results for 66 isoparaffins of carbon number 4~9. It contains the comparison of effective carbon number n^* calculated by equation (10) (Calcd. I) with the observed value at normal boiling point, the estimated and the literature values of normal boiling point, the heat of vaporization at normal boiling point, the standard heat of vaporization, the critical temperature and the critical pressure.

In Table III, the estimated values (Calcd. I) of normal boiling point of 51 isoparaffins of C=10 and C=11 are compared with experimental data. The values (Calcd. II) estimated by the equation containing the Wiener parameters (equation 41 in P–I) are also listed in these two tables for comparison.

In Table IV, the reproducibility of the literature values attained by the recommended method is summarized. The best results obtained by the other methods are also shown in the last column of the table, from which we may conclude that the present method can be recommended as the most precise one for the estimation of the heat of vaporization at normal boiling point and the critical temperature.

For the vapor pressure curve of isoparaffins, the estimated values of general boiling point by the present method are compared with the "selected values" tabulated by API Project 44.[22] By Using the n^* value calculated from equation 11, boiling points from 10 mmHg to 1500 mmHg are read on nomogram for 32 isomers of C_4H_{10} to C_8H_{18}. The average deviation for 277 points is about 1.29°C, with the maximum deviation of 4.7°C for 2,3,4–Trimethylpentane at 1000 mmHg. Although this result is highly satisfactory, the deviation will be diminished further when we adopt the observed value of n^* at normal or general boiling point. This is the case often met with, since we have ordinarily at least one boiling point datum at hand.

Discussion

As seen in the preceding sections, the effective carbon number n^* is, as a first approximation, a constant characteristic of given isoparaffin independent of the external condition such as pressure. Using the same value of n^*, both the critical constants and the vapor pressure (including the heat of vaporization) can be evaluated with high accuracy. However, slightly different values of n^* are to be assigned for each property to obtain the closest agreement with the observed values. For instance, detailed examination of the boiling point data of isoparaffins always leads to a gradual increase in n^* with increasing temperature (cf. Table I and Fig. 1). Although the increase is negligible in most cases, there is a general tendency that the more compact the structural arrangement of carbon atoms becomes, the more the n^* depends on the temperature —— e. g., 3-Methyl-3-ethylpentane (and also in the case of other isoparaffins having quaternary carbon atoms).** If this dependence becomes large, the n^* can no longer be regarded to be a constant. Such remarkable temperature (pressure) dependence will be observed when we assign the n^* values tentatively to the derivatives of paraffin hydrocarbons such as aliphatic alcohols. Constancy of n^* is the result of parallelism between the vapor pressure curve of normal paraffins and that of the compound in question. This situation can be seen in Fig. 2, in which the vapor pressure curves of few members of normal paraffin homologue, isoparaffin and other typical aliphatic compounds are presented for comparison's sake. To correlate n^* with the molecular structure, we adopt the value at normal boiling point as reference. Accordingly, it seems more reasonable to define the effective carbon number as a special measure of the normal boiling temperature. This point will be discussed later.[26]

The effective carbon number n^* of isoparaffin is always smaller than the number of carbon atoms of the corresponding normal paraffin. This may be interpreted in terms of a decrease in the contribution of tertiary or quaternary carbon atoms to the intermolecular potential caused by the screening effect of the neighboring atoms. Thus, the n^* of 2-Methylpropane (Isobutane) and 2, 2-Dimethylbutane (Neopentane) —— the simplest compounds having tertiary and quaternary carbon atom respectively —— are 3. 72 and 4. 27 (cf. Table II) which is to be compared with their carbon number, 4 and 5. The screening

** In our previous paper P-I, 2, 2, 3, 3-Tetramethylbutane was taken inadequately as such example. It was overlooked that the extreme large pressure dependence of n^* is due to its solidification at 100. 8°C (5. 7°C lower than T_b^0).

effect of the neighboring atoms should be dependent on their arrangement, and our parameters c_2 and c_3 were introduced in order to take this dependence into account for isoparaffins other than the above two. It is shown by the experimental test that the effect of the fourth or further neighbor to the branching units is negligible, and therefore, as seen in equations 8 and 9, our correlation contains the contributions of the carbon atoms only up to the third neighbors.

These brief explanations will serve for elucidating, though qualitative, the nature of the effective carbon number and our structural parameters.

In this connection, we should like to discuss the Wiener parameters. Wiener's polarity number p and path number w[8] seem to be peculiar at first, but it will be shown that these two can skilfully describe the over-all compactness and the degree of branching in isoparaffin molecules. Although their usefulness is evident, we may indicate the following drawbacks:

1) The Wiener parameter does not distinguish all the isomers of isoparaffins, because, for higher members than Octane, some isomers whose molecular structures are entirely different from one another might have the same value of Wiener's two parameters. For example, $\Delta p = -2$ and $\Delta w = 18$ both for 4-Ethylheptane and for 2, 3-Dimethylheptane.

2) The definition of two parameters seems to be arbitrary and therefore difficult to correlate with theoretical considerations.

3) The scope of application of the Wiener parameters is limited within the paraffin hydrocarbons.

4) A large systematic deviation of predicted value from the experimental one is observed in the case of some definite types of isomers, as stated earlier. This deviation seems to be serious especially in the case that two quaternary carbons are separated by one carbon atom, for examples, as in 2, 2, 4, 4-Tetramethylpentane and 2, 2, 3, 4, 4-Pentamethylpentane.

As to the last point presented just above, the present method is also useless. Tables II and III show that the largest deviation is also observed in the case of the above two isoparaffins. Average deviation is also comparable in the case of the present method and that adopted in P-I. We do not discuss individual isoparaffins in detail here, but, it should be pointed out that an opposing deviation is observed between the isomers having comparatively simple molecular structure. For example, a large positive deviation is observed in such isomers having ethyl or propyl side chains (e. g., 3, 3-Diethylhexane or 4-*n*-Propylheptane), while a negative deviation for isomers having

adjacent methyl side chains (e. g., 2, 3, 4–Trimethylpentane). For closer reproduction of the isomeric variation of isoparaffin and other organic compounds, the more elaborate correlation should be indispensable. Owing to the lack of knowledges of the relationship between the physical properties and the intermolecular force in organic liquids, any guiding principle has not given at the present stage. However, for the practical chemical engineering purposes, the present method will be quite useful.

In conclusion, the author expresses his hearty thanks to Dr. Mikio Tamura, Professor of Kyoto University and to Dr. Michio Kurata, Assistant Professor of Kyoto University for their kind guidance and criticism.

Summary

A method for estimating the isomeric variation in the physical properties of isoparaffins is developed. In this method, the "effective carbon number", a structural constant depending on the number and the relative position of side chains is introduced. An empirical equation correlating the effective carbon number with the molecular structure of compound in terms of new structural parameters is proposed. By combining this equation with the previously presented nomogram, the accurate evaluation of the vapor pressure curve and the critical constants of isoparaffins can be made only from the knowledge of structural formula of compound.

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Added in Proof: ---- After the preparation of the manuscript, we have received a monograph by Tatevskii *et al** in which an extensive method for estimating physical properties of both normal and isoparaffins is described. Their elaborate methods, though somewhat difficult to handle, will be quite useful for the calculation of physical properties. In some cases, their results are more satisfactory than ours. However, the fundamental idea underlying their methods seems to be arbitrary and empirical.

* V. M. Tatevskii, V. A. Benderskii and S. S. Yarovoi "Rules and Methods for Calculating the Physico-Chemical Properties of Paraffinic Hydrocarbons" (English Translation edited by B. P. Mullins), Pergamon Press, 1961.

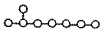
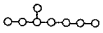
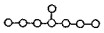
Table I. Effective Carbon Number of Isoparaffins at Various External Pressures.

Compound	Pressure (mmHg)	1	5	10	20	60	200	400	760
2-Methylpropane	T_b	−109.2	−94.1	−86.7	−77.9	−62.4	−41.5	−27.1	−11.7
	n*	3.71	3.71	3.71	3.71	3.71	3.71	3.71	3.72
2-Methylbutane	T_b	−82.9	−65.8	−57.0	−47.3	−29.4	−5.9	+10.5	27.8
	n*	4.74	4.72	4.74	4.74	4.75	4.75	4.76	4.76
2,2-Dimethylpropane	T_b	−102.0	−85.4	−76.7	−67.2	−49.0	−23.7	−7.1	+9.5
	n*	3.98	4.01	4.04	4.05	4.11	4.22	4.25	4.27
2-Methylpentane	T_b	−60.9	−41.7	−32.1	−21.4	−1.9	+24.1	41.6	60.3
	n*	5.68	5.69	5.71	5.71	5.72	5.74	5.74	5.73
3-Methylpentane	T_b	−59.0	−39.8	−30.1	−19.4	+0.1	26.5	44.2	63.3
	n*	5.76	5.77	5.79	5.79	5.80	5.82	5.82	5.82
2,2-Dimethylbutane	T_b	−69.3	−50.7	−41.5	−31.1	−12.1	+13.4	31.0	49.7
	n*	5.31	5.31	5.33	5.33	5.35	5.38	5.39	5.41
2,3-Dimethylbutane	T_b	−63.6	−44.5	−34.9	−24.1	−4.9	+21.1	39.0	58.0
	n*	5.56	5.57	5.59	5.60	5.61	5.63	5.65	5.66
2-Methylhexane	T_b	−40.4	−19.5	−9.1	+2.3	23.0	50.8	69.8	90.0
	n*	6.68	6.67	6.69	6.69	6.69	6.69	6.70	6.71
3-Methylhexane	T_b	−39.0	−18.1	−7.8	+3.6	24.5	52.4	71.6	91.9
	n*	6.74	6.74	6.74	6.74	6.75	6.75	6.77	6.77
3-Ethylpentane	T_b	−37.8	−17.0	−6.8	+4.7	25.7	53.8	73.0	93.5
	n*	6.80	6.79	6.79	6.79	6.80	6.81	6.82	6.83
2,2-Dimethylpentane	T_b	−49.0	−28.7	−18.7	−7.5	+13.0	40.3	59.2	79.2
	n*	6.24	6.26	6.27	6.27	6.29	6.31	6.33	6.34
2,3-Dimethylpentane	T_b	−42.0	−20.8	−10.3	+1.1	22.1	50.1	69.4	89.8
	n*	6.59	6.62	6.64	6.63	6.66	6.67	6.69	6.70
2,4-Dimethylpentane	T_b	−48.0	−27.4	−17.1	−5.9	+14.5	41.8	60.6	80.5
	n*	6.29	6.31	6.34	6.34	6.35	6.37	6.38	6.38
3,3-Dimethylpentane	T_b	−45.9	−25.0	−14.4	−2.9	+18.1	46.2	65.5	86.1
	n*	6.39	6.43	6.46	6.46	6.50	6.53	6.55	6.58
2,2,3-Trimethylbutane	T_b	S	S	−18.8	−7.5	+13.3	41.2	60.4	80.9
	n*	—	—	6.27	6.27	6.31	6.35	6.37	6.40

Table I. *(continued)*

Compound	Pressure (mmHg)	1	5	10	20	60	200	400	760
2-Methylheptane	T_b	−21.0	+1.3	12.3	24.4	46.6	76.0	96.2	117.6
	n*	7.64	7.66	7.66	7.66	7.68	7.68	7.70	7.73
3-Methylheptane	T_b	−19.8	+2.6	13.3	25.4	47.6	77.1	97.4	118.9
	n*	7.70	7.72	7.71	7.71	7.73	7.73	7.74	7.78
4-Methylheptane	T_b	−20.4	+1.5	12.4	24.5	46.6	76.1	96.3	117.7
	n*	7.67	7.67	7.66	7.67	7.68	7.69	7.70	7.74
2,2-Dimethylhexane	T_b	−29.7	−7.9	+3.1	15.0	36.7	65.7	85.6	106.8
	n*	7.21	7.22	7.24	7.24	7.26	7.28	7.29	7.31
2,3-Dimethylhexane	T_b	−23.0	−1.1	+9.9	22.1	44.2	73.8	94.1	115.6
	n*	7.54	7.54	7.55	7.56	7.57	7.60	7.62	7.65
2,4-Dimethylhexane	T_b	−26.9	−5.7	+5.2	17.2	39.0	68.1	88.2	109.4
	n*	7.35	7.34	7.33	7.34	7.35	7.37	7.39	7.41
2,5-Dimethylhexane	T_b	−26.7	−5.5	+5.3	17.2	38.5	68.0	87.9	109.1
	n*	7.36	7.35	7.33	7.34	7.34	7.36	7.37	7.40
3,3-Dimethylhexane	T_b	−25.8	−4.4	+6.1	18.2	40.4	70.0	90.4	112.0
	n*	7.40	7.39	7.37	7.38	7.40	7.44	7.47	7.51
3,4-Dimethylhexane	T_b	−22.1	+0.2	11.3	23.5	45.8	75.6	96.0	117.7
	n*	7.58	7.61	7.61	7.62	7.65	7.67	7.69	7.74
3-Ethylhexane	T_b	−20.0	+2.1	12.8	25.0	47.1	76.7	97.0	118.5
	n*	7.69	7.70	7.69	7.69	7.71	7.71	7.73	7.77
2,2,3-Trimethylpentane	T_b	−29.0	−7.1	+3.9	16.0	38.1	67.8	88.2	109.8
	n*	7.25	7.26	7.27	7.28	7.31	7.36	7.39	7.43
2,2,4-Trimethylpentane	T_b	−36.5	−15.0	−4.3	+7.5	29.1	58.1	78.0	99.2
	n*	6.87	6.89	6.90	6.91	6.94	6.98	7.00	7.03
2,3,3-Trimethylpentane	T_b	−25.8	−3.9	+6.9	19.2	41.8	72.0	92.7	114.8
	n*	7.40	7.41	7.41	7.42	7.47	7.52	7.56	7.62
2,3,4-Trimethylpentane	T_b	−26.3	−4.1	+7.1	19.3	41.6	71.3	91.8	113.5
	n*	7.38	7.40	7.42	7.42	7.46	7.50	7.52	7.57
2-Methyl-3-ethylpentane	T_b	−24.0	−1.8	+9.5	21.7	43.9	73.6	94.0	115.6
	n*	7.49	7.51	7.53	7.54	7.56	7.59	7.61	7.65
3-Methyl-3-ethylpentane	T_b	−23.9	−1.4	+9.9	22.3	45.0	75.3	96.2	118.3
	n*	7.50	7.53	7.55	7.56	7.61	7.66	7.70	7.76
2,2,3,3-Tetramethylbutane	T_b	−17.4	+3.2	13.5	24.6	44.5	70.2	87.4 S	106.3
	n*	7.83	7.75	7.72	7.67	7.59	7.45	7.35	7.30

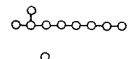
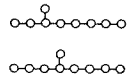
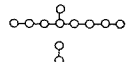
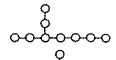
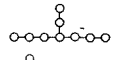
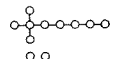
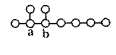
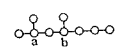
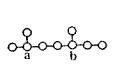
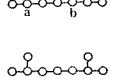
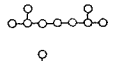
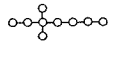
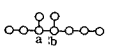
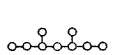
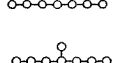
Table II. Comparison of Values of Physical Properties Estimated by Recommended.

Compound		Structural Parameters				Effective Carbon Number		n*	Normal Boiling Point $T°_b$ (°C)	
Name	Structural Pattern	C_2	C_3	$\triangle p$	$\triangle w$	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I
C_4 2-Methylpropane		0	0	1	1	3.72	3.72	3.61	−11.7	−11
C_5 2-Methylbutane		1	0	0	2	4.76	4.78	4.73	+27.8	+28
2,2-Dimethylpropane		0	0	2	4	4.27	4.27	4.10	9.5	10
C_6 2-Methylpentane		1	1	0	3	5.73	5.72	5.72	60.3	60
3-Methylpentane		2	0	−1	4	5.82	5.84	5.82	63.3	63
2,2-Dimethylbutane		1	0	0	7	5.41	5.41	5.34	49.7	49
2,3-Dimethylbutane		2 2	0a 0b	−1	6	5.66	5.68	5.61	58.0	58
C_7 2-Methylhexane		1	1	0	4	6.71	6.72	6.72	90.0	90
3-Methylhexane		2	1	−1	6	6.77	6.78	6.76	91.9	92
3-Ethylpentane		3	0	−2	8	6.83	6.90	6.81	93.5	95
2,2-Dimethylpentane		1	1	0	10	6.34	6.36	6.31	79.2	79
2,3-Dimethylpentane		2 3	1a 0b	−2	10	6.70	6.68	6.67	89.8	89
2,4-Dimethylpentane		1 1	2 2	0	8	6.38	6.32	6.45	80.5	78
3,3-Dimethylpentane		2	0	−2	12	6.58	6.55	6.53	86.1	85
2,2,3-Trimethylbutane		2 3	0a 0b	−2	14	6.40	6.45	6.39	80.9	82
C_8 2-Methylheptane		1	1	0	5	7.73	7.72	7.73	117.6	117
3-Methylheptane		2	1	−1	8	7.78	7.78	7.76	118.9	119
4-Methylheptane		2	2	−1	9	7.74	7.72	7.70	117.7	117
2,2-Dimethylhexane		1	1	0	13	7.31	7.36	7.31	106.8	108
2,3-Dimethylhexane		2 3	1a 1b	−2	14	7.65	7.62	7.62	115.6	114
2,4-Dimethylhexane		1 2	2a 2b	−1	13	7.41	7.38	7.49	109.4	109
2,5-Dimethylhexane		1 1	1 1	0	10	7.40	7.44	7.47	109.1	110
3,3-Dimethylhexane		2	1	−2	17	7.51	7.50	7.46	112.0	111
3,4-Dimethylhexane		3 3	1 1	−3	16	7.74	7.68	7.69	117.7	117
3-Ethylhexane		3	1	−2	12	7.77	7.84	7.72	118.5	121

Method with Experimental Data (I) Isoparaffins of $C_4H_{10} \sim C_9H_{20}$.

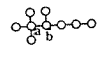
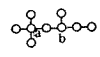
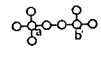
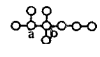
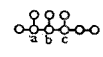
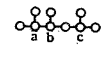
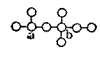
	Heat of Vaporization at Normal Boiling Point Δ° (Kcal/mol)			Standard Heat of Vaporization Δ_{25} (Kcal/mol)			Critical Temperature Tc (°K)			Critical Pressure Pc (atm)		
Calcd. II	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. II	Calcd. II	Obsd.	Calcd. I	Calcd. II
−15	5.089	5.05	4.96	4.570	4.56	4.38	408.2	410	401	36	37	38
+27	5.842	5.92	5.88	5.878	5.96	5.95	461.0	455	457	32.9	34	35
3	5.438	5.52	5.36	5.205	5.32	5.33	433.8	436	428	31.6	34	37
60	6.626	6.70	6.71	7.138	7.20	7.22	498.1	497	497	30	30	30
63	6.758	6.79	6.78	7.235	7.35	7.35	504.4	502	500	30.8	30	30
47	6.355	6.45	6.38	6.617	6.80	6.70	489.4	485	482	30.7	32	32
56	6.595	6.67	6.62	6.960	7.15	7.10	500.4	496	492	31.0	30	31
90	7.35	7.41	7.42	8.318	8.40	8.40	531.1	532	531	27.2	28	27
91	7.42	7.46	7.46	8.385	8.48	8.45	535.6	534	533	28.1	27	27
92	7.44	7.53	7.47	8.419	8.58	8.48	540.8	538	534	28.6	27	27
78	6.98	7.16	7.12	7.751	7.96	7.91	520.9	520	518	28.4	28	28
89	7.30	7.38	7.38	8.184	8.34	8.34	537.8	532	530	29.2	28	28
82	7.10	7.13	7.22	7.860	7.92	8.07	520.3	518	522	27.4	29	28
84	7.07	7.28	7.29	7.892	8.16	8.18	536	527	526	—	28	28
80	6.94	7.22	7.18	7.657	8.07	8.00	531.5	523	521	29.8	28	28
117	8.03	8.03	8.04	9.483	9.44	9.45	561	563	562	24.8	25	25
118	8.14	8.08	8.07	9.520	9.52	9.51	565	565	563	25.6	25	25
117	8.100	8.03	8.02	9.482	9.44	9.45	563	563	562	25.6	25	26
107	7.73	7.80	7.77	8.912	9.08	9.03	552	552	550	25.6	26	26
114	8.02	7.97	7.97	9.271	9.32	9.34	566	561	558	26.6	26	26
111	7.82	7.82	7.88	9.026	9.10	9.19	555	553	555	25.8	26	26
111	7.84	7.85	7.87	9.048	9.14	9.19	550	555	555	25.0	26	26
110	7.82	7.88	7.86	8.971	9.19	9.15	564	557	555	27.2	26	26
117	8.02	8.01	8.01	9.315	9.42	9.44	571	563	562	27.4	25	25
117	8.19	8.11	8.03	9.475	9.58	9.45	567	567	562	26.4	25	25

Table II. (*continued*)

	Compound		Structural Parameters				Effective Carbon Number n*			Normal Boiling Point T_b° (°C)	
	Name	Structural Pattern	C_2	C_3	Δp	Δw	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I
	2,2,3-Trimethylpentane		2 4	1a 0b	−3	21	7.43	7.46	7.42	109.8	110
	2,2,4-Trimethylpentane		1 1	2a 3b	0	18	7.03	6.91	7.04	99.2	95
	2,3,3-Trimethylpentane		3 3	1a 0b	−4	22	7.62	7.53	7.55	114.8	112
	2,3,4-Trimethylpentane		2 4 2	2a 0b 2c	−3	19	7.57	7.40	7.53	113.5	109
	2-Methyl-3-ethylpentane		2 4	2a 0b	−3	17	7.65	7.68	7.64	115.6	117
	3-Methyl-3-ethylpentane		3	0	−4	20	7.76	7.69	7.66	118.3	117
	2,2,3,3-Tetramethylbutane		3 3	0 0	−4	26	7.30	7.38	7.34	106.3	109
C_9	2-Methyloctane		1	1	0	26	8.71	8.72	8.75	143.3	143
	3-Methyloctane		2	1	−1	10	8.75	8.78	8.74	144.2	145
	4-Methyloctane		2	2	−1	12	8.69	8.72	8.68	142.5	143
	3-Ethylheptane		3	1	−2	16	8.70	8.84	8.69	143.0	146
	4-Ethylheptane		3	2	−2	18	8.67	8.78	8.60	141.2	145
	2,2-Dimethylheptane		1	1	0	16	8.23	8.36	8.33	132.7	134
	2,3-Dimethylheptane		2 3	1a 1b	−2	18	8.62	8.62	8.60	140.5	141
	2,4-Dimethylheptane		1 2	2a 3b	−1	18	8.32	8.32	8.42	133	133
	2,5-Dimethylheptane		1 2	1a 1b	−1	16	8.43	8.50	8.51	136	138
	2,6-Dimethylheptane		1 1	1 1	0	12	8.41	8.44	8.50	135.2	136
	3,3-Dimethylheptane		2	1	−2	22	8.49	8.50	8.44	137.3	138
	3,4-Dimethylheptane		3 3	1a 2b	−3	22	8.62	8.62	8.62	140.6	141
	3,5-Dimethylheptane		2 2	2 2	−2	20	8.43	8.44	8.52	136.0	136
	4,4-Dimethylheptane		2	2	−2	24	8.41	8.45	8.35	135.2	136
	2-Methyl-3-ethylhexane		2 4	2a 1b	−3	24	8.51	8.62	8.53	138.0	141

Heat of Vaporization at Normal Boiling Point Δ° (Kcal/mol)				Standard Heat of Vaporization Δ_{25} (Kcal/mol)			Critical Temperature Tc (°K)			Critical Pressure Pc (atm)		
Calcd. II	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I	Calcd. II
109	7.69	7.87	7.84	8.823	9.16	9.12	567	555	554	28.2	26	27
99	7.41	7.53	7.62	8.396	8.58	8.75	544.1	539	543	25.5	27	26
112	7.78	7.91	7.93	8.895	9.23	9.28	576	558	558	29.0	26	26
112	7.81	7.83	7.92	9.012	9.11	9.26	568	553	557	27.6	26	27
115	7.96	8.01	7.98	9.270	9.42	9.37	568	563	560	27.4	25	26
116	7.91	8.02	8.00	9.080	9.43	9.40	578	564	561	28.9	25	25
107	7.56	7.82	7.80	10.24s	9.10	9.05	544	553	552	24.5	26	27
144	8.76	8.64	8.66	10.67	10.52	10.55	—	589	591	—	23	23
144	8.79	8.68	8.65	10.69	10.62	10.54	—	590	591	—	23	23
142	8.75	8.64	8.62	10.69	10.52	10.49	—	589	588	—	23	23
142	8.78	8.72	8.62	10.71	10.67	10.48	—	591	589	—	23	23
140	8.76	8.68	8.58	10.71	10.62	10.40	—	590	587	—	23	23
133	8.31	8.42	8.41	10.10	10.15	10.11	—	580	580	—	24	24
140	8.63	8.58	8.58	10.46	10.43	10.40	—	586	587	—	23	23
135	8.45	8.39	8.46	10.25	10.10	10.19	—	578	582	—	24	24
138	8.51	8.52	8.52	10.25	10.33	10.33	—	583	584	—	24	24
138	8.49	8.49	8.52	10.24	10.25	10.30	—	581	584	—	24	24
136	8.44	8.52	8.47	10.19	10.33	10.21	—	583	583	—	24	24
141	8.69	8.58	8.59	10.48	10.43	10.44	—	586	587	—	23	23
139	8.52	8.48	8.53	10.27	10.23	10.34	—	581	585	—	24	24
134	8.45	8.49	8.42	10.19	10.25	10.12	—	582	582	—	24	24
139	8.60	8.58	8.53	10.48	10.43	10.34	—	586	585	—	23	24

Table II. (*continued*)

Compound		Structural Parameters				Effective Carbon Number n*			Normal Boiling Point T_b° (°C)	
Name	Structural Pattern	C_2	C_3	△p	△w	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I
2-Methyl-4-ethylhexane		1 3	2a 2b	−2	22	8.35	8.44	8.44	133.8	136
3-Methyl-3-ethylhexane		3	1	−4	28	8.62	8.64	8.54	140.6	141
3-Methyl-4-ethylhexane		3 4	2a 1b	−4	26	8.61	8.68	8.63	140.4	142
2,2,3-Trimethylhexane		2 4	1a 1b	−3	28	8.36	8.40	8.36	134	135
2,2,4-Trimethylhexane		1 2	2a 3b	−1	26	8.07	7.97	8.09	126.5	125
2,2,5-Trimethylhexane		1 1	1a 1b	0	22	7.99	8.08	8.08	124.1	127
2,3,3-Trimethylhexane		3 3	1a 1b	−4	30	8.50	8.48	8.46	137.7	138
2,3,4-Trimethylhexane		2 4 3	2a 1b 2c	−4	28	8.56	8.40	8.54	139.0	135
2,3,5-Trimethylhexane		2 3 1	1a 2b 2c	−2	24	8.26	8.22	8.35	131.3	131
2,4,4-Trimethylhexane		1 2	3a 2b	−2	28	8.23	8.05	8.18	130.6	126
3,3,4-Trimethylhexane		3 4	1a 1b	−5	32	8.61	8.54	8.56	140.5	139
3,3-Diethylpentane		4	0	−6	32	8.83	8.83	8.74	146.2	146
2,2-Dimethyl-3-ethylpentane		2 5	2a 0b	−4	32	8.35	8.47	8.38	133.8	137
2,3-Dimethyl-3-ethylpentane		3 4	2a 0b	−6	34	8.67	8.61	8.65	142	141
2,4-Dimethyl-3-ethylpentane		2 5 2	3a 0b 3c	−4	30	8.46	8.34	8.46	136.7	134
2,2,3,3-Tetramethylpentane		3 4	1a 0b	−6	38	8.60	8.47	8.48	140.3	137
2,2,3,4-Tetramethylpentane		2 5 2	2a 0b 3c	−4	34	8.32	8.13	8.29	133.0	128
2,2,4,4-Tetramethylpentane		1 1	3 3	0	32	7.91	7.52	7.66	122.3	113
2,3,3,4-Tetramethylpentane		3 4 3	2a 0b 2c	−6	36	8.65	8.49	8.57	141.6	138

Heat of Vaporization at Normal Boiling Point Δ° (Kcal/mol)				Standard Heat of Vaporization Δ_{25} (Kcal/mol)			Critcal Temperature Tc (°K)			Critical Pressure Pc (atm)		
Calcd. II	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. II	Calcd. II	Obsd.	Calcd. I	Calcd. II
136	8.52	8.48	8.47	10.27	10.23	10.21	—	581	583	—	24	24
139	8.54	8.59	8.54	10.28	10.44	10.35	—	587	586	—	23	23
141	8.70	8.62	8.59	10.50	10.50	10.44	—	588	587	—	23	23
134	8.31	8.46	8.43	10.02	10.21	10.13	—	580	582	—	24	24
127	8.13	8.18	8.25	9.69	9.76	9.84	—	569	573	—	24	24
127	8.07	8.25	8.25	9.601	9.87	9.84	—	571	573	—	24	24
136	8.31	8.50	8.48	10.09	10.30	10.23	—	583	583	—	24	24
139	8.53	8.46	8.54	10.26	10.21	10.34	—	580	586	—	24	23
134	8.32	8.33	8.42	9.900	10.01	10.12	—	575	582	—	24	24
129	8.20	8.23	8.31	9.76	9.82	9.92	—	571	577	—	24	24
139	8.40	8.53	8.55	10.11	10.33	10.36	—	585	586	—	23	23
144	8.60	8.71	8.65	10.36	10.66	10.54	—	591	591	—	23	23
134	8.32	8.48	8.44	10.04	10.26	10.14	—	583	582	—	24	24
141	8.44	8.58	8.60	10.17	10.43	10.45	—	586	587	—	23	23
136	8.46	8.42	8.48	10.26	10.14	10.23	—	579	583	—	24	24
137	8.43	8.48	8.50	9.80	10.26	10.27	—	583	584	—	24	24
132	8.19	8.27	8.38	9.80	9.89	10.05	—	573	579	—	24	24
115	7.85	7.90	8.00	9.11	9.26	9.38	—	556	561	—	26	25
140	8.35	8.52	8.55	9.98	10.33	10.38	—	583	586	—	24	23

Table III. Comparison of Values of Physical Properties Estimated by the Recommended Method with Experimental Data (II) Isoparaffins of $C_{10}H_{22}$ and $C_{11}H_{24}$.

Compound		Structural Parameters				Effective Carbon Number n*			Normal Boiling Point T°b (°C)		
	Name	C_2	C_3	△P	△W	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I	Calcd. II
C_{10}	2-Methylnonane	1	1	0	7	9.70	9.72	9.73	166.8	166	166
	3-Methylnonane	2	1	−1	12	9.74	9.78	9.74	167.8	168	167
	4-Methylnonane	2	2	−1	15	9.65	9.72	9.67	165.7	166	165
	5-Methylnonane	2	2	−1	16	9.63	9.72	9.64	165.1	166	164
	2,2-Dimethyloctane	1	1	0	19	—	9.36	9.35	—	158	158
	2,3-Dimethyloctane	2 1a 3 1b		−2	22	9.59	9.62	9.63	164.3	164	164
	2,4-Dimethyloctane	1 2a 2 3b		−1	23	9.12	9.32	9.40	153.2	157	159
	2,5-Dimethyloctane	1 1a 2 2b		−1	22	9.36	9.44	9.43	159	160	160
	2,6-Dimethyloctane	1 1a 2 1b		−1	19	9.41	9.50	9.53	160	161	162
	2,7-Dimethyloctane	1 1 1 1		0	14	9.41	9.44	9.54	160.2	160	162
	3,3-Dimethyloctane	2	1	−2	27	9.46	9.50	9.44	161.2	161	160
	3,4-Dimethyloctane	3 1a 3 2b		−3	28	—	9.62	9.59	—	164	163
	3,6-Dimethyloctane	2 1 2 1		−2	24	9.44	9.56	9.54	160.8	162	162
	4,5-Dimethyloctane	3 2 3 2		−3	30	9.45	9.56	9.52	161.0	162	162
	4-n-Propylheptane	3	3	−2	27	9.48	9.72	9.44	161.7	166	160
	4-Isopropylheptane	4	2	−3	34	9.35	9.56	9.38	158.6	162	159
	2-Methyl-5-ethylheptane	1 1a 3 1b		−2	27	9.33	9.56	9.44	158.4	162	160
	3-Methyl-3-ethylheptane	3	1	−4	36	9.24	9.64	9.50	156.3	164	161
	2,2,4-Trimethylheptane	1 2a 2 4b		−1	34	8.86	8.91	9.02	147	148	150
	2,2,6-Trimethylheptane	1 1a 1 1b		0	26	8.93	9.08	9.12	148.9	152	153
	2,3,3-Trimethylheptane	3 1a 3 1b		−4	38	9.41	9.48	9.43	160	161	160

Table III. (*continued*)

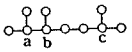
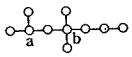
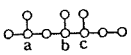
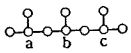
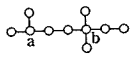
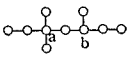
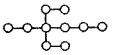
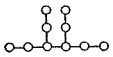
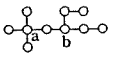
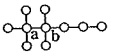
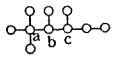
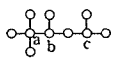
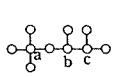
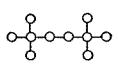
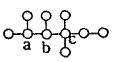
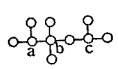
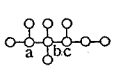
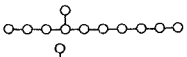
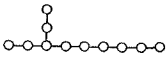
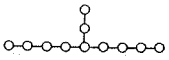
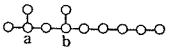
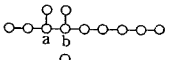
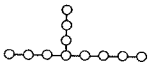
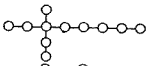
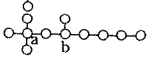
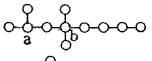
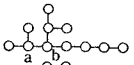
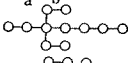
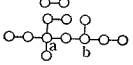
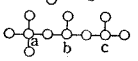
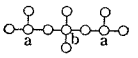
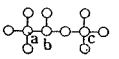
Compound		Structural Parameters				Effective Carbon Number n*			Normal Boiling Point T°b (°C)		
Name	Structural Pattern	C_2	C_3	ΔP	ΔW	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I	Calcd. II
2, 3, 6-Trimethylheptane		2 1a 3 1b 1 1c		−2	29	9.20	9.34	9.37	155.3	157	158
2, 4, 4-Trimethylheptane		1 3a 2 3b		−2	38	9.03	9.00	9.07	151	150	152
2, 4, 5-Trimethylheptane		1 2a 3 3b 3 1c		−3	35	—	9.22	9.35	—	155	157
2, 4, 6-Trimethylheptane		1 2a 2 4b 1 2c		−1	30	8.88	8.92	9.16	147.6	148	154
2, 5, 5-Trimethylheptane		1 1a 2 1b		−2	34	9.11	9.22	9.20	152.8	155	155
3, 3, 5-Trimethylheptane		2 2a 2 3b		−3	39	9.27	9.11	9.21	156.8	153	155
3, 3-Diethylhexane		4	1	−5	44	9.52	9.78	9.40	162.7	168	158
3, 4-Diethylhexane		4 2 4 2		−5	40	9.44	9.68	9.54	160.7	165	163
2, 2-Dimethyl-4-ethyl-hexane		1 2a 3 3b		−2	39	9.80	9.03	9.03	148	151	151
2, 2, 3, 3-Tetramethylhexane		3 1a 4 1b		−6	50	9.42	9.42	9.38	160.3	159	158
2, 2, 3, 4-Tetramethylhexane		2 2a 5 1b 3 3c		−5	47	9.25	9.13	9.30	156.5	153	157
2, 2, 3, 5-Tetramethylhexane		2 1a 4 2b 1 2c		−3	42	8.91	9.00	9.11	148.4	150	155
2, 2, 4, 5-Tetramethylhexane		1 2a 3 3b 2 1c		−2	41	8.81	8.81	8.97	145.8	145	145
2, 2, 5, 5-Tetramethylhexane		1 1 1 1		0	38	8.49	8.72	8.71	137.5	143	143
2, 3, 3, 4-Tetramethylhexane		3 2a 4 1b 4 2c		−7	50	9.65	9.40	9.56	165.7	159	162
2, 3, 3, 5-Tetramethylhexane		3 1a 3 2b 1 3c		−4	45	9.11	9.03	9.40	153	151	158
2, 3, 4, 4-Tetramethylhexane		2 3a 5 1b 3 2c		−6	49	9.52	9.21	9.41	162.8	155	158

Table III. (*continued*)

Compound		Structural Pattern	Structural Parameters				Effective Carbon Number n*			Normal Boilng Point T°b (°C)		
	Name		C_2	C_3	△P	△W	Obsd.	Calcd. I	Calcd. II	Obsd.	Calcd. I	Calcd. II
	2, 3, 4, 5-Tetramethylhexane		2 2a 4 2b		−5	44	9.19	9.12	9.40	155	153	158
	3, 3, 4, 4-Tetramethylhexane		4 1 4 1		−8	54	9.84	9.84	9.60	170.0	169	164
	3-Isopropyl-2, 4-dimethylpentane		2 4a 6 0b		−5	48	9.27	8.88	9.27	157.0	147	157
	3-Ethyl-2, 3, 4-trimethylpentane		3 3a 5 0b 3 3c		−8	53	9.71	9.41	9.64	167	159	164
	2, 2, 3, 3, 4-Pentamethylpentane		3 2a 5 0b 3 3c		−8	57	9.67	9.38	9.50	166.1	158	161
	2, 2, 3, 4, 4-Pentamethylpentane		2 3a 6 0b 2 3c		−5	54	9.38	8.98	9.06	159.3	149	151
C_{11}	4-Methyldecane		2	2	−1	18	10.63	10.72	10.67	188.1	188	187
	3-Ethylnonane		3	1	−2	24	—	10.84	10.65	—	191	186
	5-Ethylnonane		3	2	−2	32	—	10.78	10.46	—	190	184
	2, 4-Dimethylnonane		1 2a 2 3b		−1	28	9.93	10.32	10.39	172	180	182
	3, 4-Dimethylnonane		3 1a 3 2b		−3	34	—	10.62	10.53	—	186	186
	4-n-Propyloctane		3	3	−2	36	10.03	10.72	10.31	175.0	188	180
	3-Methyl-3-ethyloctane		3	1	−4	44	10.53	10.64	10.48	187.5	187	184
	2, 2, 4-Trimethyloctane		1 2a 2 4b		−1	42	9.88	9.91	10.00	171.5	171	173
	2, 4, 4-Trimethyloctane		2 3a 1 3b		−2	48	—	10.00	9.97	—	173	172
	3-Isopropyl-2-methylheptane		2 3a 5 1b		−4	52	9.93	10.28	10.26	172	179	178
	3, 3-Diethylheptane		4	1	−6	56	10.57	10.78	10.51	186.7	190	186
	3-Ethyl-3, 5-dimethylheptane		3 2a 2 3b		−5	58	10.26	10.25	10.27	180	178	179
	2, 2, 4, 6-Tetramethylheptane		1 2a 2 5b 1 2c		−1	50	9.50	9.51	9.77	162.2	162	167
	2, 4, 4, 6-Tetramethylheptane		1 3a 2 4b		−2	56	—	9.55	9.75	—	163	167
	2, 2, 3, 5, 5-Pentamethylhexane		2 1a 4 3b 1 2c		−3	64	9.66	9.59	9.74	166.0	164	167

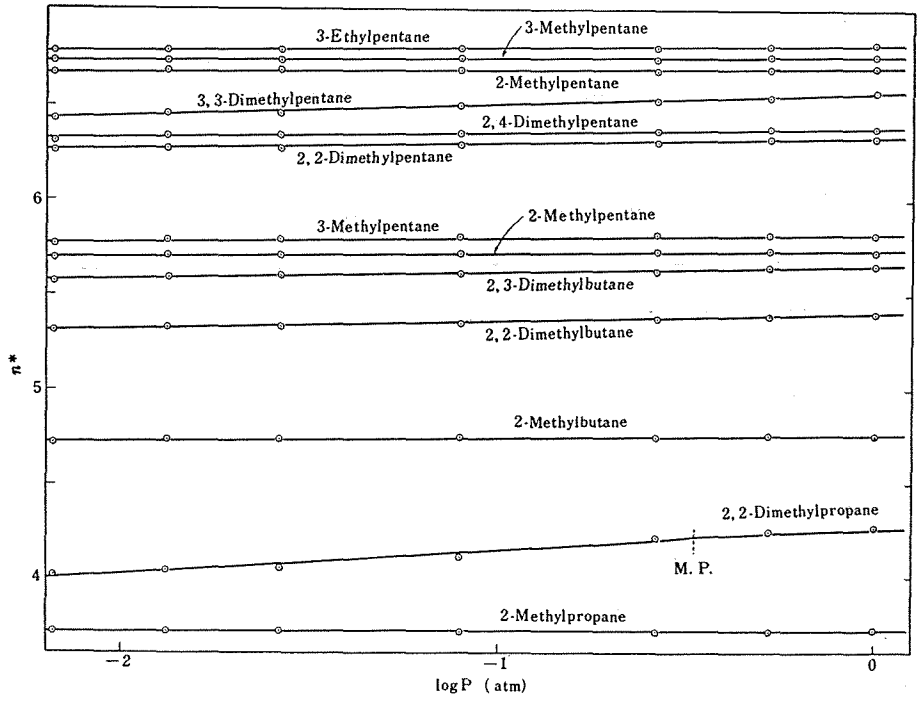


Fig. 1. Effective Number of Carbon Atoms *versus* Pressure Relation.

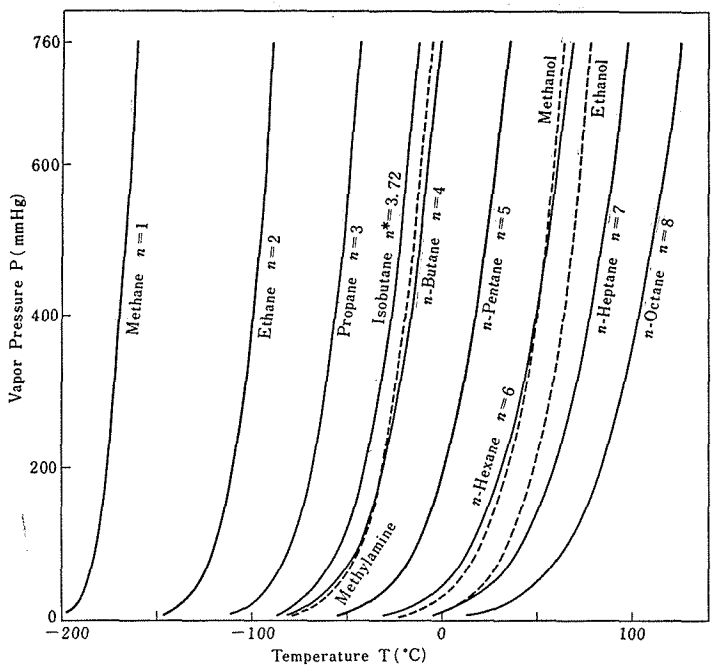


Fig. 2. Vapor Pressure Curve of Organic Compound.

Table IV. Physical Constants of Isoparaffins: Experimental Test of Recommended Method.

	Present method				Other methods		
Property	Range	No. of compd.	Average dev.	Maximum dev.	Reference	Average dev.	No. of compd.
Normal boiling point	C_4 to C_8	32	±1.2°	−5°	Wiener(8)	±1.0°	94
	C_9	34	±2.0°	−9°			
	C_{10}	41	±3.2°	−10°	Greenshields & Rossini(20)	±1.1°	103
	C_{11}	10	±3.1°	+8°			
Heat of vaporization at normal boiling point	C_4 to C_8	32	±0.09kcal/mole ±1.2%	+0.28 kcal/mole	Nakanishi, Kurata & Tamura(19)	±1.2°	66
	C_9	34	±0.08kcal/mole ±0.9%	+0.19 kcal/mole			
Standard heat of vaporization at 25°	C_4 to C_8	31	±0.15kcal/mole ±1.8%	+0.41 kcal/mole	Greenshields & Rossini(20)	±0.06 kcal/mole	30
	C_9	34	±0.13kcal/mole ±1.3%	+0.46 kcal/mole			
Critical temperature	C_4 to C_8	32	±5.0° ±0.93%	−18°	Thodos (18)	±5.2°	19
Critical pressure	C_4 to C_8	32	±1.2atm. ±4.3%	−4 atms.	Thodos (18)	±0.6 atm.	19