Estimation of Critical Temperature, Critical Pressure, and Normal Boiling Point of Alkanes and Alkenes

Toshihiko HIAKI^{†1)*}, Ichiro ANAZAWA^{†1)}, and Kazuo KOJIMA^{†2)}

^{†1)} Dept. of Industrial Chemistry, College of Industrial Technology, Nihon University,
1-2-1 Izumi-cho, Narashino-shi, Chiba 275

^{†2)} Dept. of Industrial Chemistry, College of Science and Technology, Nihon University,
1-8 Surugadai, Kanda, Chiyoda-ku, Tokyo 101

(Received July 10, 1989)

A simple and accurate method was developed, based exclusively on molecular weight and structure, to estimate the critical temperature, critical pressure, and normal boiling point of alkanes and alkenes including their isomers. With the proposed method, these properties can be calculated for 20 *n*-alkanes of carbon from 1 to 20, 44 branched alkanes of carbon from 4 to 10, sixteen 1-alkenes of carbon from 2 to 18, and 20 alkenes, other than 1-alkene of carbon from 4 to 8. A comparison of the results obtained by this method with those by conventional estimation methods is also presented.

1. Introduction

Critical temperature and pressure are essential physical properties for the development and design of chemical processes. Thus, various methods^{1)~4), 6), 8), 9), 15)} for estimating these properties have been proposed. In order to estimate these properties of hydrocarbons, including branched alkanes, it is necessary to identify and distinguish their isomers. Thus, many of the conventional methods have introduced normal boiling point as one of the variables.

This paper proposes a method for estimating critical temperatures and pressures and normal boiling points of alkanes and alkenes as functional forms consistent with their molecular weight and structure. A comparison of the estimated values obtained by the present method with those by conventional methods is also presented.

2. Functional Form of Estimation Equation

In this estimation method, critical temperature and pressure are calculated by use only the molecular weight, *M*, of *n*-alkanes and 1-alkenes. The general functional form is given by Eq. (1).

$$Q_n = A + B/M^{0.8} + C \cdot (\ln M)/M^{0.8} + D \cdot (\ln M)^{1.5}/M^{0.8} + E \cdot (\ln M)^2/M^{0.8} \quad (1)$$

where Q_n represents either the critical temperature or critical pressure of *n*-alkane or 1-alkene whose

molecular weight is *M*, and *A* to *E* are the constants which will be shown below.

For branched alkanes (*i*-alkanes) and alkenes (except 1-alkenes and *cis*-alkenes), a general form of Eq. (2) is employed.

$$Q_i = Q_n + [F + G \cdot (p_n - p_i) + H\{0.8 \cdot (p_n - p_i) + (w_n - w_i)\}/M^2] \quad (2)$$

where Q_i represents either the critical temperature or pressure of *i*-alkane or *i*-alkene (except 1-alkene and *cis*-alkene), and Q_n is the calculated value of the corresponding *n*-alkane or 1-alkene given by Eq. (1).

In addition, the Platt number, $p^{11)}$, and the Wiener number, $w^{16)}$, are introduced to distinguish between the isomers. Those numbers are calculated based on the structural formula of the molecule. In the original reports, both numbers have been defined for alkanes. Therefore, these numbers are extended to alkenes in this study (see **Appendix**).

The values of critical temperature and pressure and normal boiling point used in this work are obtained from a data base of Reid, Prausnitz, and Poling.¹³⁾

3. Estimation of Critical Temperature

3.1 *n*-Alkanes

Values of *A* to *E* in Eq. (1) were determined by fitting the critical temperatures of 20 *n*-alkanes of carbon from 1 to 20. The critical temperature of *n*-alkane, $T_{c,n}$, can be expressed by Eq. (3).

* To whom correspondence should be addressed.

$$\begin{aligned} T_{c,n} = & 1289.558 - 26646.223/M^{0.8} \\ & + 32373.522 \cdot (\ln M)/M^{0.8} \\ & - 17414.799 \cdot (\ln M)^{1.5}/M^{0.8} \\ & + 934.002 \cdot (\ln M)^2/M^{0.8} \end{aligned} \tag{3}$$

The average and maximum absolute deviations between the values calculated by Eq. (3) and those observed are shown in **Table 1**. This table shows also the deviations between the values calculated by using some of the conventional estimation methods and those observed. The results from Eq. (3) are found to be most accurate.

3.2 Branched Alkanes (*i*-alkanes)

On the basis of the observed values of critical temperature for 44 branched alkanes of carbon from 4 to 10, constants, *F* to *H*, in Eq. (2) were determined. The estimation equation for critical temperature of *i*-alkane, *T_{c,i}*, is given by Eq. (4).

$$\begin{aligned} T_{c,i} = & T_{c,n} + [-3.9376 - 7.6628 \cdot (p_n - p_i) \\ & - 16253.6123 \{0.8 \cdot (p_n - p_i) + (w_n \\ & - w_n)\}/M^2] \end{aligned} \tag{4}$$

where *T_{c,n}* is the critical temperature of *n*-alkane calculated using Eq. (3). Deviations of the values estimated by Eq. (4) from those observed are shown in **Table 1**, which includes the deviations from the values estimated by the conventional methods. Although the present equation includes only the molecular weight as a variable, it is shown to reproduce the observed values, within the allowable limits of deviation, comparable with those obtained by the Ambrose method that includes two variables: the normal boiling point and the Platt number.

3.3 Alkenes

There are three types of estimation equation for alkenes, *i.e.*, for the 1-alkenes, *cis*-alkenes, and other alkenes.

For 1-alkene, values of *A* to *E* in Eq. (1) were determined on the basis of the observed values of sixteen 1-alkenes of carbon from 2 to 18 (except C₁₆). The estimation equation thus obtained is given by Eq. (5).

$$\begin{aligned} T_{c,1\text{-alkene}} = & 1192.700 - 62597.783/M^{0.8} \\ & + 88924.776 \cdot (\ln M)/M^{0.8} \\ & - 56795.098 \cdot (\ln M)^{1.5}/M^{0.8} \\ & + 8885.519 \cdot (\ln M)^2/M^{0.8} \end{aligned} \tag{5}$$

For alkenes, except 1-alkenes and *cis*-alkenes, the estimation equation of critical temperature, derived by fitting the observed values, is given by Eq. (6).

$$\begin{aligned} T_{c,i\text{-alkene}} = & T_{c,1\text{-alkene}} + [4.1776 - 1.4034 \\ & \cdot (p_n - p_i) - 13830.0233\{0.8 \\ & \cdot (p_n - p_i) + (w_n - w_i)\}/M^2] \end{aligned} \tag{6}$$

The estimation equation for *cis*-alkenes was derived by fitting the observed values for 4 *cis*-alkenes.

$$T_{c,cis} = T_{c,i\text{-alkene}} + 16.78 - 0.22 \cdot M \tag{7}$$

Deviations of the values estimated by Eqs. (5) to (7) from the observed values are shown in **Table 1**, which includes also the deviations resulted from using previous methods. For the critical temperature of 1-alkene, the present method using Eq. (5) gives an average absolute deviation of 0.7 K and a maximum absolute deviation of 2.1 K.

For alkenes, other than 1-alkene, the method using Eqs. (6) and (7) yields an average absolute deviation of 3.5 K and a maximum absolute deviation of 10.7 K.

Table 1 Comparison of Estimation Results of Critical Temperature between This Study and Previous Methods for Alkanes and Alkenes

Author	Applying range of estimation	Deviation (K)				Applying range of estimation	Deviation (K)			
		<i>n</i> -Alkene		Branched alkane			1-Alkene		Except 1-alkene	
		AAD	MAD	AAD	MAD		AAD	MAD	AAD	MAD
This work	C ₁ —C ₂₀	0.7	2.1	1.4	4.2	C ₂ —C ₁₈	0.7	2.1	3.5	10.7
	Jalowka and Daubert (1986)	C ₂ —C ₁₃	2.0	6.6	1.4	6.9	C ₂ —C ₁₃	1.8	4.6	6.7
Klincewicz and Reid (1984)	C ₂ —C ₁₀	4.4	9.4	3.0	9.6	C ₂ —C ₁₀	4.5	13.0	4.5	14.6
Lin and Chao (1984)	C ₁ —C ₂₀	1.2	3.9	9.0	42.5	C ₂ —C ₁₈	1.8	10.1	10.6	20.8
Fedors (1982)	C ₂ —C ₂₀	1.6	9.1	9.3	41.8	C ₂ —C ₁₈	2.4	13.6	5.9	15.0
Ambrose (1974)	C ₁ —C ₂₀	0.9	4.2	0.7	3.0	C ₂ —C ₁₈	1.9	9.0	5.6	12.0
Stiel and Thodos (1962)	C ₃ —C ₁₀	2.6	9.9	2.3	7.5					
Forman and Thodos (1958)	C ₂ —C ₁₅	5.3	14.0	11.5	81.2	C ₂ —C ₁₅	3.9	10.0	5.6	14.4
Lydesen (1955)	C ₂ —C ₂₀	3.6	8.7	3.0	12.2	C ₂ —C ₁₈	2.9	6.1	7.2	17.9

AAD (average absolute deviation): (Σ|*T_{c,cal}* - *T_{c,obs}*)/*N*, *N*: number of data, MAD: maximum absolute deviation

4. Estimation of Critical Pressure

4.1 *n*-Alkanes

Values of A to E in Eq. (1) for estimating the critical pressure of *n*-alkane were determined by fitting the observed data. The equation for estimating the critical pressure of *n*-alkane, $P_{c,n}$, is given by Eq. (8).

$$P_{c,n} = -2.325 - 508.355/M^{0.8} + 736.225 \cdot (\ln M)/M^{0.8} - 481.175 \cdot (\ln M)^{1.5}/M^{0.8} + 97.839 \cdot (\ln M)^2/M^{0.8} \quad (8)$$

Deviations of the values estimated by Eq. (8) from the observed values are shown in **Table 2**, which includes also the deviations observed by the previous methods. The results estimated by Eq. (8) are more accurate than any of the conventionally estimated ones.

4.2 Branched Alkanes (*i*-alkanes)

The equation for estimating the critical pressure of *i*-alkanes, $P_{c,i}$, is given by Eq. (9).

$$P_{c,i} = P_{c,n} + [-0.0100 - 0.0636 \cdot (p_n - p_i) + 28.8562\{0.8 \cdot (p_n - p_i) + (w_n - w_i)\}/M^2] \quad (9)$$

The resulting deviations by Eq. (9) are shown in **Table 2**.

4.3 Alkenes

The equation for estimating the critical pressure of 1-alkenes was similarly derived as it was for *n*-alkanes, using only their molecular weights, as in Eq. (1). The critical pressure of 1-alkene, $P_{c,1\text{-alkene}}$, is given by Eq. (10).

$$P_{c,1\text{-alkene}} = -3.471 - 899.812/M^{0.8} + 1326.702 \cdot (\ln M)/M^{0.8} - 882.730 \cdot (\ln M)^{1.5}/M^{0.8} + 177.499 \cdot (\ln M)^2/M^{0.8} \quad (10)$$

For alkenes, except 1-alkene and *cis*-alkene, the equation derived from their observed critical pressures is developed into Eq. (11).

$$P_{c,i\text{-alkene}} = P_{c,1\text{-alkene}} + [0.0028 - 0.0310 \cdot (p_n - p_i) - 55.6782\{0.8 \cdot (p_n - p_i) + (w_n - w_i)\}/M^2] \quad (11)$$

For *cis*-alkenes, their critical pressure can be expressed by Eq. (12)

$$P_{c,cis} = P_{c,i\text{-alkene}} + 0.41 - 0.0048 \cdot M \quad (12)$$

Table 2 shows the deviations of the values estimated by Eqs. (10) to (12) and those observed, including the results estimated by the conventional methods. The average absolute deviation for 1-alkenes is found to be 0.016 MPa and the maximum absolute deviation 0.036 MPa. For alkenes, except 1-alkenes, the present method gives an absolute deviation of 0.048 MPa and a maximum absolute deviation of 0.150 MPa.

5. Equation for Estimating Normal Boiling Points of Alkanes and Alkenes

Estimation of the normal boiling point, T_b , was also attempted in a manner similar to that used for critical temperature and pressure. The equation for estimating the normal boiling point of an *n*-alkane, $T_{b,n}$, is given by Eq. (13).

$$T_{b,n} = 1563.217 + 25843.400/M^{0.8} - 76703.381 \cdot (\ln M)/M^{0.8} + 69616.048 \cdot (\ln M)^{1.5}/M^{0.8} - 19241.408 \cdot (\ln M)^2/M^{0.8} \quad (13)$$

For branched alkanes, the value of T_b is expressed by Eq. (14).

$$T_{b,i} = T_{b,n} + [-0.5205 - 5.5056 \cdot (p_n - p_i) - 19163.8056 \cdot (w_n - w_i)/M^2] \quad (14)$$

Table 2 Comparison of Estimation Results of Critical Pressure between This Study and Previous Methods for Alkanes and Alkenes

Author	Applying range of estimation	Deviation (K)				Applying range of estimation	Deviation (K)			
		<i>n</i> -Alkane		Branched alkane			1-Alkene		Except 1-alkene	
		AAD	MAD	AAD	MAD		AAD	MAD	AAD	MAD
This work	C ₁ —C ₂₀	0.017	0.045	0.027	0.066	C ₂ —C ₁₈	0.016	0.036	0.048	0.150
Jalowka and Daubert (1986)	C ₂ —C ₂₀	0.044	0.110	0.035	0.133	C ₂ —C ₁₈	0.049	0.143	0.076	0.353
Lin and Chao (1984)	C ₂ —C ₂₀	0.023	0.116	0.176	0.404	C ₂ —C ₁₈	0.084	0.238	0.181	0.443
Ambrose (1974)	C ₁ —C ₂₀	0.057	0.426	0.015	0.046	C ₂ —C ₁₈	0.075	0.283	0.099	0.230
Steil and Thodos (1962)	C ₃ —C ₁₀	0.043	0.133	0.054	0.223					
Forman and Thodos (1958)	C ₂ —C ₁₅	0.031	0.063	0.129	0.534	C ₂ —C ₁₅	0.032	0.073	0.088	0.418
Lydesen (1955)	C ₂ —C ₂₀	0.038	0.146	0.115	0.377	C ₂ —C ₁₈	0.081	0.312	0.096	0.184

AAD (average absolute deviation): $(\sum |P_{c,cal} - P_{c,obs}|)/N$, N : number of data, MAD: maximum absolute deviation

Table 3 Comparison of Estimation Result of Normal Boiling Point between This Study and Previous Methods for Alkanes and Alkenes

Author	Applying range of estimation	Deviation (K)				Applying range of estimation	Deviation (K)			
		<i>n</i> -Alkane		Branched alkane			1-Alkene		Except 1-alkene	
		AAD	MAD	AAD	MAD		AAD	MAD	AAD	MAD
This work	C ₁ —C ₂₀	0.3	0.9	0.6	2.5	C ₂ —C ₁₈	0.2	0.4	4.0	11.3
Lai, Chen and Maddox (1987)	C ₂ —C ₂₀	6.5	11.4	5.2	13.1	C ₂ —C ₁₈	5.3	18.1	6.4	27.9
Purarelli (1976)	C ₁ —C ₂₀	7.2	35.1	7.5	31.2	C ₂ —C ₁₈	1.6	17.6	6.9	22.4
Steil and Thodos (1962)	C ₃ —C ₁₀	0.1	0.2	0.7	3.1					
Ogata and Tsuchida (1957)	C ₁ —C ₇	8.5	41.8							
Somayajulu and Palit (1957)	C ₁ —C ₂₀	1.8	3.9							
Kinney (1940)	C ₁ —C ₂₀	1.9	6.8	2.7	16.2	C ₂ —C ₁₈	1.7	3.1	2.8	12.0

AAD (average absolute deviation): $(\sum |T_{b,cal} - T_{b,obs}|)/N$, N : number of data, MAD: maximum absolute deviation

The results of average absolute deviation from the observed values are listed in **Table 3**. Deviations estimated by the conventional methods are also given in this table. The results from Eqs. (13) and (14) are most accurate.

The equation for estimating the normal boiling point of alkenes is developed in a manner similar to that for estimating the critical temperature and critical pressure. The equation for 1-alkene, $T_{b,1-alkene}$, is given by Eq. (15).

$$T_{b,1-alkene} = 1499.731 - 13791.427/M^{0.8} - 15160.900 \cdot (\ln M)/M^{0.8} + 27455.613 \cdot (\ln M)^{1.5}/M^{0.8} - 10972.085 \cdot (\ln M)^2/M^{0.8} \quad (15)$$

For *i*-alkenes, except 1-alkenes and *cis*-alkenes, Eq. (16) is used.

$$T_{b,i-alkene} = T_{b,1-alkene} + [1.1267 - 0.9285 \cdot (p_n - p_i) - 13624.6156 \cdot (w_n - w_i)/M^2] \quad (16)$$

Estimation for *cis*-alkenes is given by Eq. (17).

$$T_{b,cis} = T_{b,i-alkene} + 15.94 - 0.22 \cdot M \quad (17)$$

Deviations from the observed values are shown in **Table 3**. The table also includes the deviations calculated by the conventional estimation methods^{5), 7), 10), 12), 14), 15)}.

Appendix

Calculation of the Platt Number and the Wiener Number

The Platt number, p , is indicated as the number of pairs of carbon atoms three bond apart (*i.e.* C—C—C—C). For example, for compound, *n*-hexane (C₆), the Platt number $p=3$. For 2,3-

dimethyl butane (C₆), $p=4$.

n-Hexane

2,3-Dimethyl butane

In this study the Platt number is extended to alkenes. For alkenes, the double bond is defined as two carbon—carbon bonds, and the Platt number p is counted. For example, for compound 1-hexene, $p=4$, or for 2,3-dimethyl-1-butene, $p=6$.

1-Hexene

2,3-Dimethyl-1-butene

The Wiener number, w , is calculated by multiplying the number of carbon atoms on one

side of each carbon-carbon bond by the number of carbons on the other side of the bond and adding all the contributions from each carbon-carbon bond in the structural formula. For *n*-hexane, *w*=35, or for 2,3-dimethyl butane, *w*=29; the procedure is as follows.

n-Hexane

	a : 1×5=5
	b : 2×4=8
CH ₃ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -CH ₃	c : 3×3=9
a b c d e	d : 4×2=8
	e : 5×1=5
	<hr/>
	w=35

2,3-Dimethyl butane

CH ₃ CH ₃	a : 1×5=5
b d	b : 1×5=5
CH ₃ -CH-CH-CH ₃	c : 3×3=9
a c e	d : 1×5=5
	e : 5×1=5
	<hr/>
	w=29

On the other hand, the Wiener number of alkenes is employed in a manner similar to the Platt number. Therefore, for 1-hexene, *w*=40, or for 2,3-dimethyl-1-butene, *w*=34.

1-Hexene

	a : 1×5=5
	b : 1×5=5
a	c : 2×4=8
CH ₂ =CH-CH ₂ -CH ₂ -CH ₂ -CH ₃	d : 3×3=9
b c d e f	e : 4×2=8
	f : 5×1=5
	<hr/>
	w=40

2,3-Dimethyl-1-butene

CH ₃ CH ₃	a : 1×5=5
a c e	b : 1×5=5
CH ₂ =C-CH-CH ₃	c : 1×5=5
b d f	d : 3×3=9
	e : 1×5=5
	f : 5×1=5
	<hr/>
	w=34

Nomenclatures

- A, B, C, D, E* : constants in Eq. (1)
F, G, H : constants in Eq. (2)
M : molecular weight
p_i : the Platt number of *i*-alkane or alkene (except 1-alkene)
p_n : the Platt number of *n*-alkane or 1-alkene
P_c : critical pressure
T_b : normal boiling point
T_c : critical temperature
w_i : the Wiener number of *i*-alkane or alkene (except 1-alkene)
w_n : the Wiener number of *n*-alkane or 1-alkene

References

1) Ambrose, D., Broderick, B. E., Townsend, R., *J. Appl. Chem. Biotechnol.*, **24**, 359 (1974).
2) Fedors, R. F., *Chem. Eng. Comm.*, **16**, 149 (1982).
3) Forman, J. C., Thodos, G., *AIChE J.*, **4**, 356 (1958).
4) Jalowka, J. W., Daubert, T. E., *Ind. Eng. Chem. Process Des. Dev.*, **25**, 139 (1986).
5) Kinney, C. R., *Ind. Eng. Chem.*, **32**, 559 (1940).
6) Klinecicz, K. M., Reid, R. C., *AIChE J.*, **30**, 137 (1984).
7) Lai, W. Y., Chen, D. H., Maddox, R. N., *Ind. Eng. Chem. Res.*, **26**, 1072 (1987).
8) Lin, H. M., Chao, K. C., *AIChE J.*, **30**, 981 (1984).
9) Lydesen, A. L., *Univ. of Wisconsin, Eng. Exp. Sta. Rep., Madison*, **1955**.
10) Ogata, Y., Tsuchida, M., *Ind. Eng. Chem.*, **49**, 415 (1957).
11) Platt, J. R., *J. Phys. Chem.*, **56**, 328 (1952).
12) Purarelli, C., *Chem. Eng.*, **30**, 127 (1976).
13) Reid, R. C., Prausnitz, J. M., Poling, B. E., "The Properties of Gases and Liquids, fourth edition", McGraw-Hill, New York (1986).
14) Somayajulu, G. R., Palit, S. R., *J. Chem. Soc.*, **1957**, 2540.
15) Stiel, L. I., Thodos, G., *AIChE J.*, **8**, 527 (1962).
16) Wiener, H., *J. Am. Chem. Soc.*, **69**, 17 (1947).

要 旨

アルカンおよびアルケンの臨界温度、臨界圧力ならびに標準沸点の推算

日秋 俊彦^{†1)}, 穴澤 一郎^{†1)}, 小島 和夫^{†2)}¹⁾ 日本大学生産工学工業化学科, 275 千葉県習志野市泉町 1-2-1²⁾ 日本大学理工学部工業化学科, 101 東京都千代田区神田駿河台 1-8

臨界温度、臨界圧力は化学プロセスの解析や設計に必須の物性である。したがって、臨界温度、臨界圧力については各種の推算法^{1)~4),6),8),9),15)}が提案されているが、*i*-アルカンを含め広く炭化水素の推算を行うためには異性体を区別する必要がある、このため標準沸点が多くの場合用いられている。本研究は物質の分子量と化学構造のみに基づいてアルカンおよびアルケンの臨界温度、臨界圧力および標準沸点の推算法を示し、既往の方法による推算結果と比較検討したものである。

まず *n*-アルカン、1-アルケンの臨界温度、臨界圧力および標準沸点の基本推算式として分子量 M のみを含む Eq. (1) を採用した。また *i*-アルカンならびに 1-アルケン以外のアルケン (*cis*-アルケンを除く) の基本推算式は、化学構造式に基づいて計算する Platt 数 p および Wiener 数 w を含む Eq. (2) を採用し、*cis*-アルケンに対しては分子量のみを含む式を用いた。本研究で用いたアルカンおよびアルケンの臨界温度、臨界圧力ならびに標準沸点の実測値はすべて Reid, Prausnitz および Poling の成書¹³⁾のデータベースを使用した。

20 種の *n*-アルカン ($C_1 \sim C_{20}$) および 44 種の *i*-アルカン ($C_4 \sim C_{10}$) の臨界温度データを用いて Eq. (1) および Eq. (2) のパラメーターを決定した。*n*-アルカンおよび *i*-アルカンの臨界温度の推算式を Eqs. (3), (4) に示す。推算値と実測値との絶対算術平均偏差はそれぞれ 0.7 K, 1.4 K, 最大偏差

は 2.1 K, 4.2 K であった。また 16 種の 1-アルケン ($C_2 \sim C_{18}$, C_{16} を除く) および 20 種の 1-アルケン以外のアルケン ($C_4 \sim C_8$) の臨界温度データに基づいて Eq. (1) および Eq. (2) のパラメーターを決定した。1-アルケンおよび 1-アルケン以外のアルケンの臨界温度の推算式を Eqs. (5)~(7) に示す。推算値と実測値との絶対算術平均偏差はそれぞれ 0.7 K, 3.5 K, また最大偏差 2.1 K, 10.7 K であった。同様にして Eqs. (1), (2) を用いて臨界圧力の推算を行った。*n*-アルカンおよび *i*-アルカンの臨界圧力の推算式を Eqs. (8), (9) に、1-アルケンおよび 1-アルケン以外のアルケンの推算式を Eqs. (10)~(12) に示す。*n*-アルカンおよび *i*-アルカンの推算値と実測値との絶対算術平均偏差はそれぞれ 0.017 MPa, 0.027 MPa, 最大偏差は 0.045 MPa, 0.066 MPa であった。1-アルケンおよび 1-アルケン以外のアルケンは絶対算術平均偏差はそれぞれ 0.016 MPa, 0.048 MPa であった。また標準沸点の推算も同様にして行った。*n*-アルカンおよび *i*-アルカンの標準沸点の推算式 Eqs. (13), (14), 1-アルケンおよび 1-アルケン以外のアルケンの推算式を Eqs. (15)~(17) に示す。*n*-アルカンおよび *i*-アルカンの推算値と実測値との絶対算術平均偏差が 0.3 K, 0.6 K, 最大偏差は 0.9 K, 2.5 K, 1-アルケンおよび 1-アルケン以外のアルケンでは絶対算術平均偏差はそれぞれ 0.2 K, 4.0 K, 最大偏差が 0.4 K, 11.3 K であった。

Keywords

Estimation equation, Critical temperature, Critical pressure, Normal boiling point, Alkane, Alkene