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Position Group Contribution Method for the Prediction of Critical Temperatures of Organic Compounds

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Based on position group contribution additivity, a new simple and reliable method is proposed for the prediction of critical temperatures of organic compounds involving a carbon chain from C2 to C18. Contributions for organic compounds containing oxygen, nitrogen, chlorine, bromine, and sulfur are given. The overall average absolute difference for critical temperature T_c predictions of 467 organic compounds is 6.6 K and 1.1 %, which means absolute relative difference, which is compared to 17.6 K and 3.1 % with the method of Joback and Reid and 13.5 K and 2.3 % with the method of Constantinou and Gani. Owing to the utilization of the position compensation factor, this method demonstrates significant improvements compared to the previously used first- or second-order method, especially in the capability of distinguishing between isomers. Furthermore, this new position contribution group method with better precision and simplicity is fully predictive.

Introduction

Because the experimental measurement of thermophysical properties is an expensive and time-consuming procedure, the alternative is to develop models from which the required properties with the desired accuracy could be obtained.

Group contribution methods are widely used to predict a variety of thermodynamic properties (e.g., vapor pressure, critical temperature, critical pressure, boiling point) of organic compounds. A large variety of group contribution methods have been designed in the past years, differing in their field of applicability and in the set of experimental data they are based on.[1] According to the complexity of the decomposition used to represent the molecule, the numerous group contribution methods have been classified by Benson as zero-order methods, first-order methods, and second-order methods.[2] However, most of the group contribution methods have a serious problem that they cannot distinguish among structural isomers. To overcome this problem, many researchers have tried to improve group contribution methods.

Based on conjugate forms, Constantinou et al. proposed a quite complex estimation technique, which could provide accurate estimations of several properties of pure compounds and allow capturing the differences among isomers.[3,4] However, the generation of conjugate forms is a nontrivial issue and requires a symbolic computing environment.[5] A less complex method has been proposed by Constantinou and Gani,[6] which performs the estimation at two levels: the basic level uses contributions from first-order simple groups, while the second level uses a small set of second-order groups having the first-order groups as building blocks. The role of the second-order groups is to consider the proximity effects and to distinguish among isomers. Marrero-Morejón and Pardillo-Fontdevilla proposed another technique that considers the contributions of interactions between bonding groups instead of the contributions of simple groups, which allows the distinction between isomers.[7] Dalmazzone et al.[8] reported a second group contribution method shown as formula (1) to predict the critical temperature of organics based on Benson's second-order group contribution, where A and B are obtained by summing the contributions obtained for Benson's groups that compose the molecule: $A = \sum N_iA_i$ and $B = \sum N_iB_i$. Using this method, the average differences for T_c prediction of the given 381 compounds claimed by these authors is 5.8 K, but for some compounds, the differences are very high. For example, the difference for 1-octene is 0.9 K in their work, but for *cis*-2-octene and *trans*-2-octene, the differences are up to (70.6 and 65.7) K, respectively. Furthermore, because the value of B is negative, the formula (1) could not be used for the prediction of critical temperature for the *cis*-3-octene, *trans*-3-octene, *cis*-4-octene, and *trans*-4-octene out of the samples.

$$T_c = 5.926A \cdot [0.5503 \ln B + 0.6B^2]^{-1} \tag{1}$$

The objective of this work was to develop a simple and reliable method for estimation of critical temperatures of organic compounds.

Method Proposed in this Work

Experimental Data. A total of 467 compounds were used for the determination of group contributions, which includes linear and branched alkanes (153), cycloalkanes (28), alkenes (33), aromatics (26), ketones and aldehydes (36), alcohols (34), acids (12), phenols and ether oxides (22), esters (25), bromoalkanes and chloro (18), amines and anilines (28), nitriles (9), pyridines (10), alkane thiols (16), and thio ethers (17).

The sources of experimental data were from a series of critical compilation reviews in the *Journal of Chemical and Engineering Data* by Tsonopoulos and Ambrose priority,[9,10] Daubert and Gude,[11,12] and Marsh et al.[13,14] Critical data were also obtained from a compilation of organic property data by Ma.[15]

Position Group Contributions for the Critical Temperature. The critical temperature function is constructed by all groups' contribution as well as position correction. The position

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Table 1. Position Group Contributions for the Prediction of T_C[a]

group	A/K	group	A/K
C−(CH3)(H)3	8.589	C−(C)(Br)(H)2	66.426
C−(CH2)(H)3	−3.221	C−(C)2(Br)(H)	117.880
C−(CH)(H)3	−8.890	C−(C)3(Br)	107.893
C−(C)(H)3	−14.484	C−(C)(Cl)(H)2	58.178
C−(C)2(H)2	18.079	C−(C)2(Cl)(H)	73.200
C−(C)3(H)	48.151	C−(C)3(Cl)	106.738
C−(C)4	83.076	C−(C)(Cl)2(H)	77.578
Cd−(H)(O)	46.012	C−(S)(H)3	72.873
Cd−(H)2	−27.380	C−(C)(S)(H)2	73.880
Cd−(C)(H)	−63.544	C−(C)2(S)(H)	94.062
C−(Cd)(C)(H)2	51.485	C−(C)3(S)	110.884
C−(Cd)(H)3	33.191	Cb−(N)	25.565
Cd−(C)2	−162.278	C−(N)(H)3	14.035
C−(Cd)(C)2(H)	69.961	C−(C)(N)(H)2	32.301
Cd−(Cd)(H)	108.449	C−(C)2(N)(H)	48.644
C−(Cd)(O)(H)2	89.056	C−(C)3(N)	60.814
C−(O)(H)3	34.841	C−(C)(CN)(H)2	134.543
C−(CO)(H)3	33.844	C−(C)2(CN)(H)	168.107
C−(C)(CO)(H)2	63.061	C−(C)3(CN)	195.908
C−(C)2(CO)(H)	75.234	N−(C)(H)2	219.661
C−(C)3(CO)	115.973	N−(C)2(H)	118.014
C−(C)(O)(H)2	49.710	N−(C)3	−2.076
C−(C)2(O)(H)	64.062	N−(Cb)(H)2	787.186
C−(C)3(O)	56.349	N−(Cb)(C)(H)	828.730
CO−(CH3)(O)	338.831	N−(Cb)(C)2	713.458
CO−(CH2)(O)	379.870	N_I−(Cb)2	370.289
CO−(CH)(O)	418.437	S−(C)(H)	96.099
CO−(O)(H)	448.857	S−(C)2	−159.102
CO−(C)(H)	177.738	ortho correction[b]	10.087
CO−(C)2	117.280	meta correction[b]	−2.402
CO−(Cd)(O)	715.602	cyclopentane correction	−16.667
Cb−(H)	188.476	cyclohexane correction	−5.116
Cb−(C)	−99.785	cyclopentane correction	−9.582
C−(Cb)(H)3	50.436	cyclohexane correction	15.018
C−(Cb)(C)(H)2	80.209	C_{ob}[c]	18.704
C−(Cb)(C)2(H)	103.365	C_{mb}[c]	−9.909
C−(Cb)(C)3	160.621	C_{pb}[c]	−6.961
Cb−(O)	1508.227	−(CH)< position correction	0.146
O−(Cb)(H)	−544.590	>(C)< position correction	3.971
O−(C)(H)	307.389	double bond position correction	−0.593
O−(C)2	−276.216	hydroxyl position correction	−4.667
O−(CO)(CH3)	−246.748	*trans* or *cis* structure correction	0.823
O−(CO)(CH2)	−258.532	carbonyl position correction	−7.843
O−(CO)(CH)	−238.405	Phenol position correction	0.788
O−(CO)(H)	167.195	a_2	7.723
T_O	7409.200	a_1	−6900.452

[a] Notice: The first symbol represents the element that forms the center of the group. The symbols between parentheses represent the elements to which it is linked. Usual symbols are used to represent the elements in their normal valence state. Elements in other valence states are distinguished by using additional characters; furthermore, different symbols represent multiple bonded carbons, depending on the element at the other end of the multiple bond: Cd, carbon forming a double bond with another carbon; Cb, carbon involved in a benzene or a pyridine ring; CO, C═O group; CN, C≡N group; N_I, nitrogen of the imide (C═N−) function. Also used for the nitrogen of pyridine derivatives. The pyridine ring is considered as formed of five Cb and one N_I. [b] *Ortho* and *meta* corrections consider interactions between alkyl chains through a benzene ring. [c] Corrections for pyridines: C_{ob}, C_{mb}, and C_{pb} pyridine corrections take into account alkyl ligands in positions *ortho*, *meta*, and *para* with respect to the N element, respectively.

corrections were used to take into account longer distance interaction which could distinguish most isomers including the *cis*- and *trans*- or *Z*- and *E*- structure of organic compounds for their thermodynamics properties.

Here, the critical temperature is expressed as

$$T_C - T_0 = \sum_i A_i N_i + \sum_j A_j \tanh(N_j/N) + \sum_k A_k P_k + a_1 \exp(1/M) + a_2 \exp(1/N)$$

$$N = \sum_i N_i + \sum_j N_j \quad (2)$$

Parameter A_i or A_j stands for i or j group contributions; N_i stands for the number of each group for which the carbon element forms the center of the group in the molecular formula; N_j stands for the number of each group for which the noncarbon element forms the center; N stands for the total number of groups; P_k stands for the position correlation factor; and a_1 and a_2 are parameters of the model. The set of contributions that allowed us to minimize the residual estimation difference was then computed by regression. T_0 is 7409.200 K, and M is molecular weight. Table 1 reports the values computed for the group contributions A_i.

Results and Discussion

The results of the reference compounds obtained using the new position group contribution method were presented in detail in Table 3, and the prediction computations of the critical temperature examples are shown as appendix A. Table 2 compares the critical temperature predictions obtained using our method and previous methods to experimental data. Also,

Table 2. Comparison of T_c Predicted with Our Method and with the Methods of Joback and Constantinou for Various Classes of Organic Compounds[a]

chemical family	no. of compounds	Joback		Constantinou		this work	
		MD/K	100 $\bar{\delta}$	MD/K	100 $\bar{\delta}$	MD/K	100 $\bar{\delta}$
alkanes	153	22.8	4.4	19.1	3.5	6.9	1.2
cycloalkanes	28	9.2	1.6	6.8	1.1	6.9	1.2
alkenes	33	16.5	3.2	7.8	1.5	1.9	0.3
aromatics	26	11.5	1.8	9.7	1.5	4.7	0.7
ketones and aldehydes	36	17.1	3.1	6.3	1.2	8.4	1.4
alcohols	34	17.0	3.0	12.9	2.1	8.5	1.4
acids	12	17.7	2.7	8.5	1.2	9.2	1.4
phenols and ether oxides	22	18.3	3.1	17.2	3.2	5.0	0.8
esters	25	8.2	1.5	12.5	2.3	4.6	0.8
bromo- and chloroalkanes	18	18.4	3.5	11.8	1.7	5.8	1.1
amines and anilines	28	28.0	5.7	17.3	3.2	6.6	1.3
nitriles	9	15.9	2.6	10.7	1.8	13.6	2.2
pyridines	10	17.2	2.7	23.7	3.6	3.4	0.5
alkane thiols	16	12.7	2.1	14.2	2.4	8.2	1.5
thio ethers	17	17.5	3.1	11.7	2.0	8.3	1.4
overall	467	17.6	3.1	13.5	2.3	6.6	1.1

[a] MD is the overall average absolute difference, and $\bar{\delta}$ is the average mean difference.

the overall average absolute difference (MD) between experimental and predicted values for each group of molecules, as well as the overall mean differences δ and the average mean differences $\bar{\delta}$ are summarized in Table 2.

$$\mathrm{MD} = \frac{\sum |T_{\mathrm{c,exptl}} - T_{\mathrm{c,pred}}|}{n} \tag{3}$$

$$\delta = \left| \frac{T_{\mathrm{c,exptl}} - T_{\mathrm{c,pred}}}{T_{\mathrm{c,exptl}}} \right| \tag{4}$$

$$\bar{\delta} = \frac{1}{N} \sum_{n} \left| \frac{T_{\mathrm{c,exptl}} - T_{\mathrm{c,pred}}}{T_{\mathrm{c,exptl}}} \right| \tag{5}$$

Results presented in Table 2 show that the proposed method is more accurate than other methods for the critical temperature. The MD for critical temperature T_c predictions of 467 organic compounds is 6.6 K, and the $\bar{\delta}$ is 1.1 %, which is compared to 17.6 K and 3.1 % with the method of Joback and 13.5 K and 2.3 % with the method of Constantinou and Gani.

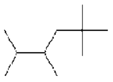
To test the quality of the regressed parameters of the position group contributions equation, the degree of confidence should be calculated. According to the definition of the F distribution function, the degree of confidence is calculated with the incomplete β function which could be calculated from the γ function. The results show that the correlation coefficient is 0.9896; the value of F distribution is 190.26; and the degree of confidence is 0.9998, which confirms the greater precision of our position group contribution method which can be used for the best estimation of the critical temperature of organic compounds.

Conclusion

A new quantitative relationship for estimating critical temperature based on position group contribution method has been proposed. Contributions for compounds containing carbon, hydrogen, oxygen, nitrogen, sulfur, chlorine, and bromine were reported, and that position compensation factor has been developed which could distinguish between the thermodynamic properties of most isomers of organic compounds including *cis-* and *trans-* or *Z-* and *E*-structures. The predicted results for 467 different organic compounds showed that the position group contribution method is more precise than the existing methods that use first- or second-order groups. Hence, using our new position group contribution method, a greater prediction precision could be obtained for organic compounds, and no extra group classification complexity was added in the process.

Appendix A

A.1. Example 1. Estimation of the critical temperature of 2,2,4,5-tetramethylhexane:



This compound is decomposed in the position groups as follows

$3\mathrm{C{-}(CH)(H)_3}$; $3\mathrm{C{-}(C)(H)_3}$; $1\mathrm{C{-}(C)_2(H)_2}$; $2\mathrm{C{-}(C)_3(H)}$; $1\mathrm{C{-}(C)_4}$

Total number of groups: $N = 10$.

The position factor: position of (CH) group 4, 5; the compensated factor is $P = 4 + 5 = 9$. Position of (C) group 2; the compensated factor is $P = 2$.

Molecular weight: $M = 142.285$.

From the contributions in Table 1, the critical temperature is estimated by eq 2

$$T_c = -8.890 \cdot 3 - 14.484 \cdot 3 + 18.079 \cdot 1 + 48.151 \cdot 2 + 83.076 \cdot 1 + 7.723 \cdot \exp(1/10) - 6900.452 \cdot \exp(1/142.285) + 0.1469 \cdot 3.971 \cdot 2 + 7409.200 = 605.2\ \mathrm{K}$$

The calculated result is 605.2 K, while the experimental critical temperature is 599.7 K.

A.2. Example 2. Estimation of the critical temperature of 2-ethyl hexanoic acid:

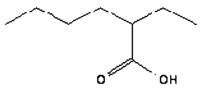


Table 3. Fully Predictive Estimations of Critical Temperature T_c^a

		this work		
compound	exptl	predict	D	100 δ
ethane	305.32	305.3	0.0	0.0
propane	369.83	356.9	12.9	3.5
n-butane	425.12	428.6	3.5	0.8
2-methylpropane	408.14	420.7	12.5	3.1
n-pentane	469.7	469.7	0.0	0.0
2-methylbutane	460.39	467.4	7.0	1.5
2,2-dimethylpropane	433.75	455.0	21.2	4.9
n-hexane	507.6	503.2	4.4	0.9
2-methylpentane	497.5	500.9	3.4	0.7
3-methylpentane	504.4	506.7	2.3	0.5
2,2-dimethylbutane	488.7	499.8	11.1	2.3
2,3-dimethylbutane	499.9	498.8	1.1	0.2
n-heptane	540.2	532.4	7.8	1.4
2-methylhexane	530.1	530.1	0.0	0.0
3-methylhexane	535.2	535.9	0.7	0.1
3-ethylpentane	540.5	541.6	1.1	0.2
2,2-dimethylpentane	520.4	528.9	8.5	1.6
2,3-dimethylpentane	537.3	533.7	3.6	0.7
2,4-dimethylpentane	519.7	528.1	8.4	1.6
3,3-dimethylpentane	536.3	544.2	7.9	1.5
2,2,3-trimethylbutane	531.1	526.8	4.3	0.8
n-octane	568.7	558.9	9.8	1.7
2-methylheptane	559.6	556.6	3.0	0.5
3-methylheptane	563.6	562.4	1.2	0.2
4-methylheptane	561.7	562.5	0.8	0.2
3-ethylhexane	565.4	568.1	2.7	0.5
2,2-dimethylhexane	549.8	555.4	5.6	1.0
2,3-dimethylhexane	563.4	560.1	3.3	0.6
2,4-dimethylhexane	553.5	560.3	6.8	1.2
2,5-dimethylhexane	550	554.8	4.8	0.9
3,3-dimethylhexane	562	570.6	8.6	1.5
3,4-dimethylhexane	568.8	566.1	2.7	0.5
2-methyl-3-ethylpentane	567	565.8	1.2	0.2
3-methyl-3-ethylpentane	576.5	581.9	5.4	0.9
2,2,3-trimethylpentane	563.4	558.9	4.5	0.8
2,2,4-trimethylpentane	543.9	553.4	9.5	1.8
2,3,3-trimethylpentane	573.5	568.4	5.1	0.9
2,3,4-trimethylpentane	566.3	558.1	8.2	1.4
n-nonane	594.6	583.5	11.1	1.9
2-methyloctane	587	581.2	5.8	1.0
4-ethyloctane	618.2	616.2	2.0	0.3
2,2-dimethyloctane	602	597.7	4.3	0.7
2,3-dimethyloctane	613	608.1	4.9	0.8
2,4-dimethyloctane	600	608.2	8.2	1.4
2,5-dimethyloctane	603	608.4	5.4	0.9
2,6-dimethyloctane	606	608.5	2.5	0.4
2,7-dimethyloctane	604	603.0	1.0	0.2
3,3-dimethyloctane	614.9	618.6	3.7	0.6
3,4-dimethyloctane	619.8	614.0	5.8	0.9
3,5-dimethyloctane	609.4	614.2	4.8	0.8
3,6-dimethyloctane	609.4	614.3	4.9	0.8
4,4-dimethyloctane	614.9	622.6	7.7	1.2
4,5-dimethyloctane	619.8	614.3	5.5	0.9
4-propylheptane	618.2	616.2	2.0	0.3
3-ethyl-2-methylheptane	619.8	613.7	6.1	1.0
3-ethyl-3-methylheptane	627.4	629.9	2.5	0.4
3-ethyl-4-methylheptane	624.2	619.7	4.5	0.7
3-ethyl-5-methylheptane	613.9	619.9	6.0	1.0
4-ethyl-2-methylheptane	609.4	613.9	4.5	0.7
4-ethyl-3-methylheptane	624.2	619.7	4.5	0.7
4-ethyl-4-methylheptane	627.4	639.4	12.0	1.9
5-ethyl-2-methylheptane	609.4	614.0	4.6	0.8
2,2,3-trimethylheptane	615.2	606.9	8.3	1.3
2,2,4-trimethylheptane	598.1	607.0	8.9	1.5
2,2,5-trimethylheptane	598.9	607.2	8.3	1.4
2,2,6-trimethylheptane	593.6	601.7	8.1	1.4
2,3,3-trimethylheptane	623.2	616.3	6.9	1.1
2,3,4-trimethylheptane	621.3	611.8	9.5	1.5
2,3,5-trimethylheptane	611	611.9	0.9	0.1
2,3,6-trimethylheptane	606.5	606.4	0.1	0.0
2,4,4-trimethylheptane	606.1	620.3	14.2	2.3
2,4,5-trimethylheptane	611	612.1	1.1	0.2
2,4,6-trimethylheptane	596.2	606.5	10.3	1.7
2,5,5-trimethylheptane	606.1	624.3	18.2	3.0
3-methyloctane	590.15	587.0	3.1	0.5
4-methyloctane	587.65	587.2	0.5	0.1
2-ethylheptane	594.3	586.9	7.4	1.2
3-ethylheptane	590.45	592.7	2.2	0.4
4-ethylheptane	594.3	592.8	1.5	0.2
2,2-dimethylheptane	576.69	580.0	3.3	0.6
2,3-dimethylheptane	591.4	584.7	6.7	1.1
2,4-dimethylheptane	581	584.9	3.9	0.7
2,5-dimethylheptane	581	585.0	4.0	0.7
2,6-dimethylheptane	577.85	579.5	1.7	0.3
3,3-dimethylheptane	591	595.3	4.3	0.7
3,4-dimethylheptane	595.8	590.7	5.1	0.9
3,5-dimethylheptane	585.5	590.9	5.4	0.9
4,4-dimethylheptane	591.4	599.2	7.8	1.3
3-ethyl-2-metylhexane	595.8	590.4	5.4	0.9
3-ethyl-3-metylhexane	603.5	606.5	3.0	0.5
3-ethyl-4-methylhexane	600.3	596.4	3.9	0.7
4-ethyl-2-methylhexane	585.5	590.6	5.1	0.9
2,2,3-trimethylhexane	591.3	583.6	7.7	1.3
2,2,4-trimethylhexane	573.55	583.7	10.2	1.8
2,2,5-trimethylhexane	569.8	578.2	8.4	1.5
2,3,3-trimethylhexane	596.05	593.0	3.1	0.5
2,3,4-trimethylhexane	597.4	588.4	9.0	1.5
2,3,5-trimethylhexane	579.15	582.9	3.8	0.6
2,4,4-trimethylhexane	581	597.0	16.0	2.7
3,3,4-trimethylhexane	602.25	598.9	3.3	0.5
3,3-diethylpentane	616	595.1	20.9	3.4
3-ethyl-2,2-dimethylpentane	595.7	589.2	6.5	1.1
3-ethyl-2,3-dimethylpentane	611.8	604.3	7.5	1.2
3-ethyl-2,4-dimethylpentane	597.4	588.4	9.0	1.5
2,2,3,3-tetramethylpentane	607.5	591.8	15.7	2.6
2,2,3,4-tetramethylpentane	574.6	581.6	7.0	1.2
2,2,4,4-tetramethylpentane	592.7	584.5	8.2	1.4
2,3,3,4-tetramethylpentane	607.1	591.0	16.1	2.7
n-decane	617.7	606.8	10.9	1.8
2-methylnonane	610	604.5	5.5	0.9
3-methylnonane	613	610.3	2.7	0.4
4-methylnonane	610	610.5	0.5	0.1
5-methylnonane	610	610.6	0.6	0.1
3-ethyloctane	618.2	616.0	2.2	0.4
3-ethyl-2,2-dimethylhexane	619.6	629.3	9.7	1.6
3-ethyl-2,3-dimethylhexane	635.7	633.2	2.5	0.4
3-ethyl-2,4-dimethylhexane	625.8	617.4	8.4	1.3
3-ethyl-2,5-dimethylhexane	611	611.9	0.9	0.1
3-ethyl-3,4-dimethylhexane	640.1	633.5	6.6	1.0
4-ethyl-2,2-dimethylhexane	602.6	612.7	10.1	1.7
4-ethyl-2,3-dimethylhexane	625.8	622.7	3.1	0.5
4-ethyl-2,4-dimethylhexane	618.6	631.5	12.9	2.1
4-ethyl-3,3-dimethylhexane	632.1	627.9	4.2	0.7
2,2,3,3-tetramethylhexane	623	615.1	7.9	1.3
2,2,3,4-tetramethylhexane	621.2	610.6	10.6	1.7
2,2,3,5-tetramethylhexane	606.4	605.1	1.3	0.2
2,2,4,4-tetramethylhexane	599.3	619.1	19.8	3.3
2,2,4,5-tetramethylhexane	599.7	605.2	5.5	0.9
2,3,3,4-tetramethylhexane	635.9	620.0	15.9	2.5
2,3,3,5-tetramethylhexane	614.4	614.5	0.1	0.0
2,3,4,4-tetramethylhexane	629.2	623.8	5.4	0.9
2,3,4,5-tetramethylhexane	622.9	609.9	13.0	2.1
3,3,4,4-tetramethylhexane	640.9	634.3	6.6	1.0
3,3-dethyl-2-methylpentane	648.2	609.6	38.6	6.0
3-ethyl-2,2,3-trimethylpentane	640.9	632.0	8.9	1.4
3-ethyl-2,2,4-trimethylpentane	621.2	610.6	10.6	1.7
3-ethyl-2,3,4-trimethylpentane	643.9	625.6	18.3	2.8
2,2,3,3,4-pentamethylpentane	636.7	618.8	17.9	2.8
2,2,3,4,4-pentamethylpentane	616.6	611.4	5.2	0.8
n-undecane	639	629.2	9.8	1.5
n-dodecane	658	650.9	7.1	1.1
n-tridecane	675	672.0	3.0	0.4
n-tetradecane	693	692.7	0.3	0.0
n-pentadecane	708	713.0	5.0	0.7
n-hexadecane	723	733.1	10.1	1.4
n-heptadecane	736	752.9	16.9	2.3
n-octadecane	747	772.6	25.6	3.4
cyclopropane	397.91	397.9	0.0	0.0

Table 3. (Continued)

		this work		
compound	exptl	predict	*D*	100 *δ*
3,3,4-trimethylheptane	627.7	622.3	5.4	0.9
3,3,5-trimethylheptane	609.6	622.4	12.8	2.1
3,4,4-trimethylheptane	627.7	626.1	1.6	0.3
3,4,5-trimethylheptane	625.8	606.5	19.3	3.1
3,4-diethylhexane	639.9	625.4	14.5	2.3
3,3-diethylhexane	628.7	641.1	12.4	2.0
cis-1,2-dimethylcyclopentane	565.15	564.4	0.8	
trans-1,2-dimethylcyclopentane	553.15	562.7	9.6	
cis-1,3-dimethylcyclopentane	551	564.5	13.5	
trans-1,3-dimethylcyclopentane	553	562.9	9.9	
1,1-dimethylcyclopentane	547	560.7	13.7	
1,1-dimethylcyclohexane	591.15	599.1	7.9	
cis-1,2-dimethylcyclohexane	606.15	602.7	3.4	
trans-1,2-dimethylcyclohexane	596.15	601.1	4.9	
cis-1,3-dimethylcyclohexane	587.7	602.9	15.2	
trans-1,3-dimethylcyclohexane	598	601.2	3.2	
cis-1,4-dimethylcyclohexane	598.15	603.0	4.9	
trans-1,4-dimethylcyclohexane	587.7	601.4	13.7	
ethylcyclohexane	609.15	604.2	5.0	
n-propylcyclopentane	596	604.2	8.2	
n-propylcyclohexane	639.15	628.9	10.2	
n-butylcyclopentane	621	617.4	3.6	
n-butylcyclohexane	667	652.4	14.6	
n-pentylcyclopentane	643.8	640.9	2.9	
n-pentylcyclohexane	669	674.9	5.9	
n-hexylcyclopentane	664.1	663.4	0.7	
n-heptylcyclohexane	682.6	685.1	2.5	
1-butene	419.5	420.0	0.5	
cis-2-butene	435.5	431.2	4.3	
trans-2-butene	428.6	429.6	1.0	
1-pentene	464.8	466.9	2.1	
cis-2-pentene	475	476.0	1.0	
trans-2-pentene	475	474.4	0.6	
2-methyl-1-butene	465	462.5	2.5	
2-methyl-2-butene	470	472.9	2.9	
3-methyl-1-butene	452.7	452.7	0.0	
1-hexene	504	504.2	0.2	
cis-2-hexene	513	514.1	1.1	
trans-2-hexene	513	512.5	0.5	
cis-3-hexene	509	510.5	1.5	
trans-3-hexene	509	508.9	0.1	
2-methyl-1-hexene	538	537.4	0.6	
3-methyl-1-hexene	528	528.0	0.0	
4-methyl-1-hexene	534	539.7	5.7	
1-heptene	537.3	536.0	1.3	
cis-2-heptene	549	546.6	2.4	
n-heptylbenzene	714	706.6	7.4	1.0
butanone	536.7	528.9	7.8	1.5
2-pentanone	561.1	556.8	4.3	0.8
3-pentanone	561.5	556.9	4.6	0.8
3-methyl-2-butanone	553	536.8	16.2	2.9
2-hexanone	587	582.5	4.5	0.8
3-hexanone	582.8	582.5	0.3	0.0
3,3-dimethyl-2-butanone	570.9	570.9	0.0	0.0
4-methyl-2-pentanone	574.6	617.2	42.6	7.4
2-heptanone	611.4	605.7	5.7	0.9
3-heptanone	606.6	605.9	0.7	0.1
4-heptanone	602	598.1	3.9	0.7
2-methyl-3-hexanone	593	585.6	7.4	1.2
2,4-dimethyl-3-pentanone	579.1	565.8	13.3	2.3
2-methyl-3-heptanone	614.9	646.3	31.4	5.1
2,5-dimethyl-3-hexanone	597.5	606.3	8.8	1.5
5-nonanone	641.4	634.5	6.9	1.1
4-nonanone	643.7	642.3	1.4	0.2
3-nonanone	648.1	650.1	2.0	0.3
2-nonanone	652.2	650.1	2.1	0.3
2,6-dimethyl-4-heptanone	619.4	638.3	18.9	3.1
6-undecanone	678.5	668.3	10.2	1.5
2-undecanone	688	691.7	3.7	0.5
3-undecanone	684.6	691.8	7.2	1.1
4-undecanone	680.9	684.0	3.1	0.5
5-undecanone	679.4	676.1	3.3	0.5
propanal	505	508.8	3.8	0.8
butanal	537	535.9	1.1	0.2
cyclobutane	459.93	459.9	0.0	0.0
cyclopentane	511.6	492.8	18.8	3.7
cyclohexane	553.5	538.8	14.7	2.7
methylcyclopentane	532.79	530.4	2.3	0.4
methylcyclohexane	572.19	571.7	0.5	0.1
ethylcyclopentane	569.5	565.8	3.7	0.6
trans-2-heptene	543	544.9	1.9	0.4
cis-3-heptene	545	543.0	2.0	0.4
trans-3-heptene	540	541.3	1.3	0.2
1-octene	566.65	564.4	2.2	0.4
cis-2-octene	572	575.5	3.5	0.6
trans-2-octene	577	573.9	3.1	0.5
cis-3-octene	569	571.9	2.9	0.5
trans-3-octene	574	570.3	3.7	0.7
cis-4-octene	568	571.3	3.3	0.6
trans-4-octene	573	569.7	3.3	0.6
1-nonene	594	590.5	3.5	0.6
1-decene	617	614.9	2.1	0.3
1-undecene	638	638.2	0.2	0.0
1-dodecene	658	660.8	2.8	0.4
1,3-butadiene	425	425.0	0.0	0.0
benzene	562.05	572.5	10.5	1.9
methylbenzene	591.75	594.2	2.5	0.4
1,4-dimethylbenzene	616.2	615.7	0.5	0.1
1,2-dimethylbenzene	630.3	625.8	4.5	0.7
1,3-dimethylbenzene	617	613.3	3.7	0.6
ethylbenzene	617.15	621.3	4.2	0.7
1,2,3-trimethylbenzene	664.5	657.3	7.2	1.1
1,2,4-trimethylbenzene	649.1	647.2	1.9	0.3
1,3,5-trimethylbenzene	637.3	632.3	5.0	0.8
1,2,3,4-tetramethylbenzene	693	692.2	0.8	0.1
1,2,3,5-tetramethylbenzene	679	679.7	0.7	0.1
1,2,4,5-tetramethylbenzene	675.15	682.1	6.9	1.0
1-methyl-2-ethylbenzene	647.2	654.1	6.9	1.1
1-methyl-3-ethylbenzene	637.2	641.6	4.4	0.7
1-methyl-4-ethylbenzene	640.2	644.0	3.8	0.6
n-propylbenzene	635.38	638.9	3.5	0.5
isopropylbenzene	631.05	629.4	1.7	0.3
1-methyl-2-isopropylbenzene	653.5	663.7	10.2	1.6
1-methyl-3-isopropylbenzene	649	651.2	2.2	0.3
1-methyl-4-isopropylbenzene	652	653.6	1.6	0.2
n-butylbenzene	660.5	656.0	4.5	0.7
sec-butylbenzene	664.54	652.2	12.4	1.9
tert-butylbenzene	660	660.0	0.0	0.0
n-pentylbenzene	679.9	672.8	7.1	1.0
n-hexylbenzene	698	689.7	8.3	1.2
1-butanol	563.05	563.1	0.1	0.0
2-butanol	536.05	545.8	9.8	1.8
2-methyl-1-propanol	547.78	560.8	13.1	2.4
2-methyl-2-propanol	506.21	505.8	0.4	0.1
1-pentanol	588.15	586.0	2.2	0.4
2-pentanol	560.3	568.7	8.4	1.5
3-pentanol	559.6	574.9	15.3	2.7
2-methyl-1-butanol	575.4	598.1	22.7	3.9
3-methyl-1-butanol	579.4	595.7	16.3	2.8
2-methyl-2-butanol	545	549.1	4.1	0.7
3-methyl-2-butanol	556.1	584.0	27.9	5.0
1,2-butanedial	680	654.3	25.7	3.8
1,3-butanedial	676	644.0	32.0	4.7
1-hexanol	610.3	607.5	2.8	0.5
2-hexanol	585.9	590.3	4.4	0.7
3-hexanol	582.4	591.3	8.9	1.5
2-methyl-1-pentanol	604.4	610.9	6.5	1.1
4-methyl-1-pentanol	603.5	605.6	2.1	0.3
2-methyl-2-pentanol	559.5	555.9	3.6	0.6
2-methyl-3-pentanol	576	558.9	17.1	3.0
4-methyl-2-pentanol	603.5	588.3	15.2	2.5
1-heptanol	632.6	628.3	4.3	0.7
2-heptanol	608.3	611.0	2.7	0.4
3-heptanol	605.4	612.0	6.6	1.1
4-heptanol	602.6	607.4	4.8	0.8
1-octanol	652.5	648.5	4.0	0.6
2-octanol	637	631.2	5.8	0.9
3-octanol	628.5	632.2	3.7	0.6

Table 3. (Continued)

		this work					this work		
compound	exptl	predict	*D*	100 δ	compound	exptl	predict	*D*	100 δ
1-pentanal	567	560.8	6.2	1.1	4-octanol	625.1	627.5	2.4	0.4
1-hexanal	592	584.2	7.8	1.3	1-nonanol	668.9	668.3	0.6	0.1
1-heptanal	617	606.5	10.5	1.7	2-nonanol	649.5	651.0	1.5	0.2
1-octanal	639	628.0	11.0	1.7	phenol	694.25	696.3	2.0	0.3
1-nonanal	659	648.8	10.2	1.5	*o*-cresol	697.6	698.7	1.1	0.2
1-decanal	674	669.2	4.8	0.7	*m*-cresol	705.7	699.5	6.2	0.9
2-methylpropanal	507	515.7	8.7	1.7	*p*-cresol	704.5	700.3	4.2	0.6
2-methylhexanal	592	604.2	12.2	2.1	2,3-xylenol	722.8	721.0	1.8	0.3
3-methylhexanal	595	610.0	15.0	2.5	2,4-xylenol	707.6	709.3	1.7	0.2
ethanol	513.92	508.8	5.2	1.0	2,5-xylenol	706.9	712.5	5.6	0.8
1-propanol	536.78	538.1	1.3	0.2	2,6-xylenol	701	710.9	9.9	1.4
2-propanol	508.3	515.1	6.8	1.3	3,4-xylenol	729.8	722.6	7.2	1.0
3,5-xylenol	715.6	710.9	4.8	0.7	butylamine	526.8	531.8	5.0	0.9
3-ethylphenol	718.8	714.3	4.5	0.6	isobutylamine	528.5	529.7	1.2	0.2
2-ethylphenol	703	713.5	10.5	1.5	*sec*-butylamine	514.3	521.2	6.9	1.3
4-ethylphenol	716.4	715.0	1.4	0.2	*tert*-butylamine	483.9	483.9	0.0	0.0
diethyl ether	466.7	462.9	3.8	0.8	diethylamine	496.6	504.6	8.0	1.6
isopropyl methyl ether	464.2	451.1	13.1	2.8	pentylamine	555	557.8	2.8	0.5
ethyl *n*-propyl ether	500.2	504.6	4.4	0.9	cyclopentylamine	582.15	576.9	5.2	0.9
butyl methyl ether	512.7	511.0	1.7	0.3	hexylamine	584	581.7	2.3	0.4
methyl pentyl ether	546.5	546.2	0.3	0.1	butyl ethylamine	547.1	551.5	4.4	0.8
butyl ethyl ether	531	539.7	8.7	1.6	isopropyl propylamine	520	542.5	22.5	4.3
dipropyl ether	530.6	539.7	9.1	1.7	triethylamine	535	519.1	15.9	3.0
diisopropyl ether	500.3	503.2	2.9	0.6	dipropylamine	550	548.9	1.1	0.2
methyl formiate	487.2	495.5	8.3	1.7	diisopropylamine	523.1	505.2	17.9	3.4
methyl acetate	506.5	500.4	6.1	1.2	cyclohexylamine	615	612.8	2.2	0.4
ethyl formiate	508.4	510.1	1.7	0.3	dibutylamine	602.3	596.0	6.3	1.0
propyl formiate	538	520.3	17.7	3.3	benzenamine	699	696.0	3.0	0.4
ethyl acetate	523.3	519.9	3.4	0.6	2-methylbenzenamine	694.15	703.0	8.8	1.3
methyl propionate	530.7	536.8	6.1	1.2	3-methylbenzenamine	709.15	703.7	5.4	0.8
propyl acetate	549.7	546.0	3.7	0.7	*N*-methylbenzenamine	698.2	700.0	1.8	0.3
isopropyl acetate	531	531.0	0.0	0.0	*N*-ethylbenzenamine	698	696.0	2.0	0.3
methyl butanoate	554.5	553.3	1.2	0.2	*N*,*N*-dimethylbenzenamine	687	687.9	0.9	0.1
methyl isobutanoate	540.7	547.1	6.4	1.2	*N*,*N*-diethylbenzenamine	689.2	688.1	1.1	0.2
2-propenyl acetate	552.2	552.2	0.0	0.0	pyridine	620	619.8	0.2	0.0
2-ethenyl acetate	525	525.0	0.0	0.0	2-methylpyridine	621	619.7	1.3	0.2
ethyl propionate	546	552.8	6.8	1.2	3-methylpyridine	645	644.3	0.7	0.1
butyl acetate	579	570.2	8.8	1.5	4-methylpyridine	645.7	648.0	2.3	0.4
propyl propionate	578	576.1	1.9	0.3	2,3-dimethylpyridine	655.7	648.3	7.4	1.1
ethyl butanoate	566	568.2	2.2	0.4	2,4-dimethylpyridine	647	651.9	4.9	0.8
n-propyl butyrate	600	590.5	9.5	1.6	2,5-dimethylpyridine	644.2	648.3	4.1	0.6
ethyl isobutanoate	553.6	555.6	2.0	0.4	2,6-dimethylpyridine	623.8	623.7	0.1	0.0
methyl pentanoate	567	568.5	1.5	0.3	3,4-dimethylpyridine	683.8	676.5	7.3	1.1
ethyl pentanoate	570	582.6	12.6	2.2	3,5-dimethylpyridine	667.2	672.9	5.7	0.8
propyl pentanoate	613	604.1	8.9	1.4	propanenitrile	561.3	526.4	34.9	6.2
diphenyl ether	766.8	766.8	0.0	0.0	butanenitrile	585.4	568.4	17.0	2.9
methylamine	430.05	411.2	18.8	4.4	2-methylpropanenitrile	569.28	569.3	0.0	0.0
dimethylamine	437	430.8	6.2	1.4	pentanenitrile	610.3	602.6	7.7	1.3
ethylamine	456.4	464.5	8.1	1.8	3-methylbutanenitrile	591.62	606.2	14.6	2.5
propylamine	497	501.9	4.9	1.0	2,2-dimethylpropanenitrile	587.61	587.6	0.0	0.0
isopropylamine	471.8	485.6	13.8	2.9	hexanenitrile	633.8	632.4	1.4	0.2
trimethylamine	433.3	442.5	9.2	2.1	octanenitrile	674.4	684.0	9.6	1.4
decanenitrile	693.2	730.1	36.9	5.3	2-propanethiol	517	527.3	10.3	2.0
chloroethane	460.35	468.6	8.3	1.8	1-butanethiol	570.1	567.0	3.1	0.5
1-chloropropane	503.1	504.1	1.0	0.2	2-butanethiol	554	560.2	6.2	1.1
2-chloropropane	482.4	486.5	4.1	0.9	2-methyl-1-propanethiol	559	564.8	5.8	1.0
1-chlorobutane	542	534.8	7.2	1.3	2-methyl-2-propanethiol	530	527.6	2.4	0.4
2-chlorobutane	520.6	522.9	2.3	0.4	1-pentanethiol	597.7	592.1	5.6	0.9
2-chloro-2-methylpropane	507	507.0	0.0	0.0	2-methyl-1-butanethiol	591.7	595.5	3.8	0.6
1-chloropentane	568	562.3	5.7	1.0	3-methyl-1-butanethiol	589.3	578.8	10.5	1.8
2-chloropentane	556.8	550.4	6.4	1.2	2-methyl-2-butanethiol	570.1	564.0	6.1	1.1
1-chloro-3-methylbutane	560	560.2	0.2	0.0	3-methyl-2-butanethiol	576.4	583.2	6.8	1.2
1,1-dichloroethane	523.4	520.1	3.3	0.6	2,2-dimethyl-1-propanethiol	574.9	588.6	13.7	2.4
bromoethane	503.9	521.1	17.2	3.4	cyclopentanethiol	633.5	615.6	17.9	2.8
1-bromopropane	536.9	544.5	7.6	1.4	1-hexanethiol	620.5	615.7	4.8	0.8
2-bromopropane	556	574.9	18.9	3.4	2-methyl-2-pentanethiol	586.3	587.5	1.2	0.2
1-bromobutane	571.1	567.5	3.6	0.6	2,3-dimethyl-2-butanethiol	599.3	585.4	13.9	2.3
1-bromo-2-methylpropane	567.2	565.2	2.0	0.4	cyclohexanethiol	664.2	651.0	13.2	2.0
2-bromo-2-methylpropane	540.5	540.5	0.0	0.0	1-heptanethiol	646	638.1	7.9	1.2
1-bromopentane	590	589.8	0.2	0.0	acetic acid	590.7	600.2	9.5	1.6
methylthio ethane	553	532.0	21.0	3.8	*n*-propanoic acid	604	618.7	14.7	2.4
1-methylthio propane	574.1	571.5	2.6	0.5	acrylic acid	615	615.0	0.0	0.0
2-methylthio propane	549.5	559.0	9.5	1.7	*n*-butyric acid	615.2	625.3	10.1	1.6
1-methylthio butane	591.3	604.8	13.5	2.3	*n*-pentanoic acid	643	636.3	6.7	1.0

Table 3. (Continued)

		this work		
compound	exptl	predict	D	100 δ
2-methyl-2-methylthio propane	569.8	565.4	4.4	0.8
1-ethylthio propane	583.9	584.5	0.6	0.1
2-ethylthio propane	571.2	572.0	0.8	0.1
1-ethylthio butane	609.2	602.6	6.6	1.1
2-ethylthio butane	599.5	590.2	9.3	1.5
2-ethylthio-2-methyl propane	549	574.6	25.6	4.7
methylthio cyclopentane	651.3	658.0	6.7	1.0
1,2-dibromopropane	679.6	660.7	18.9	2.8
1,1,2-trichloroethane	602	605.3	3.3	0.6
methylthio methane	470	469.2	0.8	0.2
ethanethiol	499.15	509.1	10.0	2.0
1-propanethiol	536	539.7	3.7	0.7
2-ethyl butyric acid	655	646.3	8.7	1.3
2-ethyl hexanoic acid	674	675.6	1.6	0.2
n-hexanoic acid	655	649.7	5.3	0.8
n-heptanoic acid	678	664.5	13.5	2.0
n-octanoic acid	693	680.1	12.9	1.9
n-nonanoic acid	711	696.4	14.6	2.1
n-decanoic acid	726	713.0	13.0	1.8
isobutyl acetate	560.8	567.6	6.8	1.2
isobutyl acrylate	587	587.0	0.0	0.0
isobutyl butyrate	610.4	609.4	1.0	0.2
isobutyl formate	551.35	553.6	2.3	0.4

[a] D is the absolute difference. $D = |T_{c,\text{exptl}} - T_{c,\text{pred}}|$.

This compound is decomposed in the position groups as follows

$$2\text{C}-(\text{CH}_2)(\text{H})_3;\ 4\text{C}-(\text{C})_2(\text{H})_2;\ 1\text{C}-(\text{C})_2(\text{CO})(\text{H});\ 1\text{CO}-(\text{CH})(\text{O});\ 1\text{O}-(\text{CO})(\text{H})$$

Total number of groups: $N = 9$.

The position of $-(\text{CH})<$ group; the compensated factor is $P = 2$.

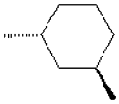
Molecular weight: $M = 144.214$.

From the contributions in Table 1, the critical temperature is estimated by eq 2

$$T_c = -3.221\cdot 2 + 18.079\cdot 4 + 75.234\cdot 1 + 418.437\cdot\tanh(1/9)\cdot 1 + 167.195\cdot\tanh(1/9)\cdot 1 + 7.723\cdot\exp(1/9) - 6900.452\cdot\exp(1/144.214) + 0.146\cdot 2 + 7409.200 = 675.6\ \text{K}$$

Therefore, the calculated result is 675.6 K, while the experimental critical temperature is 674 K.

A.3. Example 3. Estimation of the critical temperature of *trans*-1,3-dimethylcyclohexane



This compound could be decomposed in the position groups as follows

$$2\text{C}-(\text{CH})(\text{H})_3;\ 4\text{C}-(\text{C})_2(\text{H})_2;\ 2\text{C}-(\text{C})_3(\text{H})$$

Total number of groups: $N = 8$.

The position factor: position of (CH3) group 1, 3; the compensated factor is $P = 1 + 3 = 4$.

The position of the *trans*-structure compensated factor is -1.

One cyclohexane correction.

Molecular weight: $M = 112.215$.

From the contributions in Table 1, the critical temperature is estimated by eq 2

$$T_c = -8.890\cdot 2 + 18.079\cdot 4 + 48.151\cdot 2 - 5.116 + 0.146\cdot 4 + (-1)\cdot 0.823 + 7.723\cdot\exp(1/8) - 6900.452\cdot\exp(1/112.215) + 7409.200 = 601.2\ \text{K}$$

So, the calculated result is 601.2 K, while the experimental critical temperature is 598 K.

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