Prediction of the Enthalpy of Vaporization of Organic Compounds at Their Normal Boiling Point with the Positional Distributive Contribution Method

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Recently, our laboratory proposed a new universal method for the prediction of properties of organic compounds, such as the critical temperature, critical pressure, critical volume, critical compressibility factor, normal boiling point, and melting point. Here, the positional distributive contribution method is extended for the prediction of the enthalpy of vaporization of organic compounds at their normal boiling point ($\Delta_{vap}H_b$). In this method, the position factor was used to take into account longer distance interactions, which could distinguish the overall isomer including the *cis*- and *trans*- or *Z*- and *E*- structure of organic compounds for their thermodynamics properties. The results indicate that our model provides very satisfactory results. The overall average absolute difference for $\Delta_{vap}H_b$ prediction of the 311 organic compounds is 1.00 $\text{kJ}\cdot\text{mol}^{-1}$, and 2.7 % is the relative deviation. Compared to those currently used prediction methods (including Riedel, Chen, Vetere, Liu, and Joback and Reid), the new proposed method could make significant improvements both in accuracy and in stability without requiring any input property. The most important point must be claimed is that all of those properties (T_c, P_c, V_c, Z_c, T_b, and T_m) mentioned above and $\Delta_{vap}H_b$ in this work are predicted by the totally same universal positional distributive function and group framework proposed.

I. Introduction

The design of many processes in chemical engineering requires physical property data of the compounds involved. The enthalpy of vaporization at the normal boiling point ($\Delta_{vap}H_b$) is an important parameter that is utilized for the design and operation of vapor−liquid equilibrium-based processes such as distillation, evaporation, drying, and so forth. Furthermore, this property is sometimes used in the prediction or correlation of other thermodynamic properties. In spite of the increased availability of $\Delta_{vap}H_b$ experimental values, it is usually necessary to supplement data with results calculated or extrapolated by some methods.

The enthalpy of vaporization at the normal boiling point can be calculated either by quantitative structure−property relationship (QSPR) models[1] or more simply by means of empirical correlations.[2−16] According to Mohammadi and Richon,[16] these empirical correlations for the prediction of the enthalpy of vaporization are grouped into two classes. The first class is comprised of equations that relate $\Delta_{vap}H_b$ to the critical values and the normal boiling point. The second class consists of empirical correlations, which relate $\Delta_{vap}H_b$ to a few easily obtainable parameters, such as the normal boiling point, the molecular weight, and the specific gravity. Cachadina and Mulero[17] reviewed the validity of 10 different methods for the prediction of $\Delta_{vap}H_b$, six being specific models (Riedel,[7] Chen,[8] Vetere-73,[9] Vetere-79,[10] Vetere-95,[11] and Liu[12]) and four being general models (Carruth and Kobayashi (CK),[3] Sivaraman, Magee, and Kobayashi (SMK),[13] Morgan and Kobayashi (MK),[14] and Morgan (M)[15]), and the results showed that all of the models can reproduce $\Delta_{vap}H_b$ with good accuracy (AADs less than 4 %). Unfortunately, no specific or general model gives the best agreement with the DIPPR values for all of the selected fluids. Recently, combining the equations of SMK[13] correlation and M[15] correlation, Cachadina and Mulero[18] proposed a new predictive model for $\Delta_{vap}H_b$ of fluids. The main differences with respect to previous models are in the choice of the reference fluids and in the use of the analytical expression.

Also, the enthalpy of vaporization may be calculated by means of group contribution models, in which it is necessary to know the chemical groups in the molecule as well as its chemical structure. Some of them have been specifically developed to give the enthalpy of vaporization at the normal boiling point.[19−23] These methods provide the advantage of quick estimates without requiring substantial computational resources. However, most group contribution methods have a serious problem that they cannot distinguish among structural isomers and have limited applicability. To overcome these limitations, several attempts have been reported in the literature. Constantinou and Gani[24] and Marrero and Gani[25] developed methods which perform estimations at two or three levels. Also, Dalmazzone et al.[26] reported a second group contribution method to predict critical temperature and the enthalpy of vaporization of organic based on Benson's second-order group contribution (shown as eqs 1 and 2). As described in our previous work,[27] using their method, the T_c prediction 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, owing to the reason that the value of B is negative, their method could not be used for T_c predictions for the *cis*-3-octene, *trans*-3-octene, *cis*-4-octene, and *trans*-4-octene out of the samples. Therefore, on the basis of this T_c model, the enthalpy of vaporization prediction could

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Table 1. Position Group Contributions for the Prediction of $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$

group[a]	A kJ·mol^{-1}	group[a]	A kJ·mol^{-1}
C—(CH$_3$)(H)$_3$	−1.531	C—(C)$_3$(S)	11.047
C—(CH$_2$)(H)$_3$	−3.786	Cb—(N)	31.575
C—(CH)(H)$_3$	−3.859	C—(N)(H)$_3$	−6.061
C—(C)(H)$_3$	−3.218	C—(C)(N)(H)$_2$	1.148
C—(C)$_2$(H)$_2$	1.965	C—(C)$_2$(N)(H)	4.009
C—(C)$_3$(H)	6.574	C—(C)(CN)(H)$_2$	15.614
C—(C)$_4$	7.320	C—(C)$_2$(CN)(H)	17.008
Cd—(H)$_2$	−19.359	C—(C)$_3$(CN)	16.265
Cd—(C)(H)	2.315	O—(Cb)(H)	−43.926
C—(Cd)(C)(H)$_2$	0.929	O—(CH$_2$)(H)	48.022
C—(Cd)(H)$_3$	−3.440	O—(CH)(H)	41.718
Cd—(C)$_2$	17.701	O—(C)(H)	−54.808
C—(Cd)(C)$_2$(H)	5.789	O—(C)$_2$	−51.222
Cd—(Cd)(H)	−1.652	O—(CO)(CH$_3$)	67.264
Cd—Cd	0.814	O—(CO)(CH$_2$)	80.442
C—(Cd)(0)(H)$_2$	6.812	O—(CO)(CH)	92.366
C—(O—C)(H)$_3$	2.277	O—(CO)(H)	79.076
C—(O—CO)(H)$_3$	6.399	N—(CH$_3$)(H)$_2$	30.231
C—(CO)(H)$_3$	6.729	N—(CH$_2$)(H)$_2$	23.060
C—(C)(CO)(H)$_2$	14.808	N—(CH)(H)$_2$	21.773
C—(C)$_2$(CO)(H)	17.535	N—(C)(H)$_2$	52.978
C—(C)$_3$(CO)	16.383	N—(cyclohexy)(H)$_2$	4.737
C—(C)(O)(H)$_2$	7.350	N—(C)$_2$(H)	44.136
C—(C)$_2$(O)(H)	10.908	N—(C)$_3$	63.655
C—(C)$_3$(O)	11.399	N—(Cb)(H)$_2$	−151.469
C—(H)$_2$(O)$_2$	9.492	N$_{\mathrm{I}}$—(Cb)$_2$	24.589
CO—(CH$_3$)(O)	−90.521	S—(C)(H)	−1.346
CO—(CH$_2$)(O)	−75.660	Cl—	−9.680
CO—(CH)(O)	−72.650	Br—	0.451
CO—(O)(H)	−64.440	para correction[b]	2.389
CO—(C)(H)	−14.538	ortho correction[b]	0.930
CO—(C)$_2$	−43.495	meta correction[b]	1.334
C—(C)(Br)(H)$_2$	5.840	cyclopentane correction	−10.117
C—(C)$_2$(Br)(H)	10.393	cyclohexane correction	−10.444
C—(C)$_3$(Br)	8.593	C$_{\mathrm{ob}}$[c]	0.341
C—(C)(Cl)(H)$_2$	5.947	C$_{\mathrm{mb}}$[c]	1.447
C—(C)$_2$(Cl)(H)	9.624	C$_{\mathrm{pb}}$[c]	1.613
C—(C)$_3$(Cl)	11.808	cyclopropane correction	−9.470
C—(C)(Cl)$_2$(H)	11.964	cyclobutane correction	−9.787
Cb—(H)	4.460	>(CH) position factor[d]	0.247
Cb—(C)	−32.990	>(C)< position factor[d]	1.545
C—(Cb)(H)$_3$	5.438	double bond position factor[d]	1.507
C—(Cb)(C)(H)$_2$	10.454	hydroxyl position factor[d]	−0.763
C—(Cb)(C)$_2$(H)	15.151	*trans* or *cis* structure	0.227
C—(Cb)(C)$_3$	18.432	carbonyl position factor[d]	−2.780
Cb—(O)	147.145	phenol position factor[d]	−0.418
Cb—(COOH)	144.404	hydroxyl *tert*-carbon position factor[d]	8.114
Cb—(Cb)	73.205	a_2	−25.335
C—(S)(H)$_3$	1.450	a_1	55.293
C—(C)(S)(H)$_2$	5.572	$\Delta_{\mathrm{vap}}H_{\mathrm{b0}}$	2.359
C—(C)$_2$(S)(H)	9.847		

[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$_{\mathrm{I}}$, nitrogen of the imide (C═N—) function, which is also used for the nitrogen of pyridine derivatives. The pyridine ring is considered as formed of five Cb and one N$_{\mathrm{I}}$. *trans* or *cis* correction: *cis*-structure correction is 1, and *trans* structure is −1. [b] Para, ortho, and meta corrections consider interactions between alkyl chains through a benzene ring. [c] Corrections for pyridines: C$_{\mathrm{ob}}$, C$_{\mathrm{mb}}$, and C$_{\mathrm{pb}}$ pyridine corrections take into account alkyl ligands in position ortho, meta, and para with respect to the N element, respectively. [d] Position correction.

not be actualized. Also, owing to the reason that the value of β might be negative, their method could not be used for the prediction of enthalpies of vaporization for some organic compounds. For instance, the β is negative for dipropdehyde ether (COHCH$_2$CH$_2$OCH$_2$CH$_2$COH). The real solution could not be obtained if β is negative.

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

$$\Delta H_{\mathrm{vap}} = \alpha(1 - T_{\mathrm{r}})^{\sqrt{\beta - \beta\cdot T_{\mathrm{r}} + \beta\cdot T_{\mathrm{r}}^2}} \tag{2}$$

Recently, our laboratory proposed a universal model for the prediction of thermodynamic properties of organic compounds. The higher prediction accuracy of the proposed method shown in our previous works suggests that it is indeed fine to use the same framework to predict the critical properties (the critical temperature,[27] pressure,[28] volume,[29] and critical compressibility factor[30]) and the boiling point[31] and melting point temperatures[32] of organic compounds containing various functionalities.

This work is a part of ongoing investigations of thermodynamic properties of organic compounds. Therefore, the objective of this work is the application of our universal model in the prediction of the enthalpy of vaporization of organic compounds at the boiling point. Also, in this work, to evaluate the performance of our model, some other methods, including Riedel,[7] Chen,[8] Vetere,[10] Liu,[12] and Joback and Reid[19] methods are used for comparison.

II. Methods

A. Methods Used for Comparison. The most classical empirical expression is that of Riedel,[7] which requires as input parameters the critical temperature and pressure, T_{c} and P_{c}, and the normal boiling point, T_{b}.

$$\Delta_{\mathrm{vap}}H_{\mathrm{b}} = 1.093RT_{\mathrm{c}}(T_{\mathrm{b}}/T_{\mathrm{c}})\frac{\ln P_{\mathrm{c}} - 1.013}{0.930 - T_{\mathrm{b}}/T_{\mathrm{c}}} \tag{3}$$

Chen[8] presented a correlation, which was expressed by the critical pressure, the critical temperature, and the normal boiling point.

$$\Delta_{\mathrm{vap}}H_{\mathrm{b}} = RT_{\mathrm{b}}\frac{3.978(T_{\mathrm{b}}/T_{\mathrm{c}}) - 3.958 + 1.555 \ln P_{\mathrm{c}}}{1.07 - T_{\mathrm{b}}/T_{\mathrm{c}}} \tag{4}$$

The Vetere method is as follows:[10]

$$\Delta_{\mathrm{vap}}H_{\mathrm{b}} = RT_{\mathrm{b}}\frac{(1 - T_{\mathrm{b}}/T_{\mathrm{c}})^{0.38}[\ln P_{\mathrm{c}} - 0.513 + 0.5066T_{\mathrm{c}}^{\,2}/(P_{\mathrm{c}}T_{\mathrm{b}}^{\,2})]}{1 - T_{\mathrm{b}}/T_{\mathrm{c}} + [1 - (1 - T_{\mathrm{b}}/T_{\mathrm{c}})^{0.38}]\ln(T_{\mathrm{b}}/T_{\mathrm{c}})} \tag{5}$$

The Liu method is as follows:[12]

$$\Delta_{\mathrm{vap}}H_{\mathrm{b}} = RT_{\mathrm{b}}\left(\frac{T_{\mathrm{b}}}{220}\right)^{0.0627}\cdot\frac{(1 - T_{\mathrm{b}}/T_{\mathrm{c}})^{0.38}\ln(P_{\mathrm{c}}/P_{\mathrm{a}})}{1 - T_{\mathrm{b}}/T_{\mathrm{c}} + 0.38(T_{\mathrm{b}}/T_{\mathrm{c}})\ln(T_{\mathrm{b}}/T_{\mathrm{c}})} \tag{6}$$

where P_{a} is the atmospheric pressure.

The Joback and Reid method is as follows:[19]

$$\Delta_{\mathrm{vap}}H_{\mathrm{b}} = 15.30 + \sum_i n_i(\Delta H_{\mathrm{vb}})_i \qquad (7)$$

B. Experimental Data. A total of 311 compounds containing carbon, hydrogen, oxygen, nitrogen, chlorine, bromine, and sulfur were used for the determination of group contributions, which includes linear and branched alkanes (67) and cycloalkanes (31), alkenes (38), aromatics (21), ketones and aldehydes (17), alcohols (24), phenols and ether oxides (19), acids (13), esters (16), amines and pyridines (32), and nitriles and alkane thiols (33).

The sources of $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ experimental data were from the CRC Handbook of Chemistry and Physics[33] and a compilation of organic property data by Ma.[44] The sources of the critical temperature and pressure experimental data were from a series of critical compilation reviews by the critical properties group of the International Union of Pure and Applied Chemistry (IUPAC) I.2 on thermodynamics; the works were published in the *Journal of Chemical and Engineering Data* by Ambrose et al.,[34,35] Tsonopoulos et al.,[36,39,41] Gude and Teja,[37] Daubert,[38] Kudchadker et al.,[40] and Marsh et al.[42,43] Critical data were also obtained from a compilation of organic property data by Ma.[44] The sources of the boiling point experiment data were from the DIPPR database.[45]

C. Positional Distributive Contribution Method for the Enthalpy of Vaporization at the Normal Boiling Point. In this work, the specific position of a group in the molecule was considered as the position factor (P_k). The position factors were used to take into account longer distance interactions, which could distinguish the overall isomer including the *cis*- and *trans*- or *Z*- and *E*- structure of organic compounds for their thermodynamics properties. According to the IUPAC nominating method, the structures were drawn, and the relevant position factors values were assigned. The enthalpy of vaporization at the normal boiling point function is constructed by all groups' contribution as well as the position factors.

Here, the position distribution function for the prediction of $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ is expressed as eqs 8 and 9:

$$\Delta_{\mathrm{vap}}H_{\mathrm{b}} = \Delta_{\mathrm{vap}}H_{\mathrm{bo}} + \sum_i A_iN_i + \sum_j A_j \tanh(N_j/N) + \sum_k A_kP_k + a_1\exp(1/M) + a_2\exp(1/N) \qquad (8)$$

$$N = \sum_i N_i + \sum_j N_j \qquad (9)$$

Parameter A_i or A_j stands for i or j group contributions, N_i for the number of each group having a saturated carbon atom as its center in the molecular formula, N_j for the number of each of the other groups, N for total number of groups, A_k for the position factor contributions, P_k for the position factor, a_1, a_2 for parameters of the model, M for molecular weight. The hyperbolic tangent function is used especially for the groups whose center is not a saturated carbon atom. For instance, if there is a Cb—(C), Cd—Cd, or Cb—(H) group in some organic compounds, the hyperbolic tangent function should be considered.

Table 1 reports the values computed for the group contributions and the position factor contributions. Our method developed is applicable only to comparatively low molar mass compounds involving a carbon chain from C2 to C22.

III. Results and Discussion

A. Prediction of the Enthalpy of Vaporization at the Normal Boiling Point. The $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ results of the reference compounds obtained using the new positional distributive contribution method are presented in Table 4. To illustrate the application of the proposed method, a detailed procedure for the prediction of $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ is given in Appendix A. Table 2 compares $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ predictions obtained using our method and previous methods to experimental data. Also, the overall average absolute deviation (AAD) between experimental and predicted values for each group of molecules, as well as the relative deviation δ and the average relative deviation $\bar{\delta}$, are summarized

Table 3. Distribution of the Average Relative Difference $\bar{\delta}$ Obtained for All Compounds from the Basic Database

$\bar{\delta}$	Riedel[7]	Chen[8]	Vetere[10]	Liu[12]	Joback and Reid[19]	this work
≤ 1.00 %	36.66	46.30	45.34	44.69	0.64	35.69
≤ 2.00 %	53.06	62.38	63.67	67.20	2.57	53.05
≤ 3.00 %	65.60	76.21	75.89	74.60	3.21	66.23
≤ 4.00 %	74.92	81.68	83.93	79.74	4.17	77.48
≤ 5.00 %	82.32	85.22	86.18	84.56	5.46	83.91
≤ 6.00 %	86.82	88.44	87.14	87.45	6.10	88.09
≤ 7.00 %	90.04	90.69	90.36	90.02	8.35	90.02
≤ 8.00 %	91.65	91.98	91.32	90.66	9.64	92.27
≤ 9.00 %	92.61	93.59	93.25	91.30	9.96	95.49
≤ 10.00 %	92.93	94.55	93.57	92.26	10.92	97.42
> 10.00 %	7.07	5.45	6.43	7.74	89.08	2.58
overall	100.00	100.00	100.00	100.00	100.00	100.00

Table 2. Comparison of $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ Predicted with Our Method and with the Methods of Riedel,[7] Chen,[8] Vetere,[10] Liu,[12] and Joback and Reid[19] for Various Classes of Organic Compounds[a]

		Riedel[7]		Chen[8]		Vetere[10]		Liu[12]		Joback and Reid[19]		this work	
		AAD		AAD		AAD		AAD		AAD		AAD	
chemical family	samples	kJ·mol⁻¹	100 $\bar{\delta}$	kJ·mol⁻¹	100 $\bar{\delta}$	kJ·mol⁻¹	100 $\bar{\delta}$	kJ·mol⁻¹	100 $\bar{\delta}$	kJ·mol⁻¹	100 $\bar{\delta}$	kJ·mol⁻¹	100 $\bar{\delta}$
alkanes	67	0.76	1.84	0.49	1.24	0.52	1.32	0.66	1.60	11.44	29.88	0.55	1.63
cycloalkanes	31	0.98	2.40	0.66	1.76	0.55	1.49	0.45	1.16	13.97	34.69	0.40	1.10
alkenes	38	1.10	3.16	0.72	2.38	0.61	2.16	0.60	2.09	7.82	20.06	0.89	2.98
aromatics	21	1.27	2.90	1.10	2.45	1.10	2.42	1.10	2.45	16.73	43.35	1.07	2.71
ketones and aldehydes	17	0.68	2.00	0.50	1.48	0.45	1.33	0.43	1.27	11.38	33.29	1.47	4.40
alcohols	24	2.94	5.98	3.76	7.74	4.71	9.86	5.31	11.22	23.89	53.28	2.09	4.45
phenols and ether oxides	19	1.66	3.97	1.26	3.00	1.00	2.38	0.95	2.28	18.89	42.94	1.24	3.22
acids	13	10.51	27.42	14.18	35.40	3.94	11.78	3.85	11.46	19.29	48.25	1.71	4.06
esters	16	0.67	1.96	0.54	1.58	0.77	2.24	0.71	2.07	14.55	41.54	1.19	3.61
amines and pyridines	32	0.96	2.66	0.75	2.09	0.74	2.10	0.71	2.02	16.66	45.90	0.62	1.85
nitriles and alkane thiols	33	2.15	4.34	1.08	2.53	0.95	2.21	0.72	2.08	12.74	39.40	1.37	3.80
overall	311	1.65	4.01	1.54	3.80	1.15	2.91	1.18	2.98	14.18	36.81	1.00	2.74

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

Table 4. Fully Predictive Estimations of the Enthalpy of Vaporization at the Normal Boiling Point Using the Positional Distributive Contribution Method[a]

compounds	$\frac{\Delta_{\text{vap}}H_{\text{b,exp}}}{\text{kJ}\cdot\text{mol}^{-1}}$	$\frac{\Delta_{\text{vap}}H_{\text{b,pred}}}{\text{kJ}\cdot\text{mol}^{-1}}$	D	$100\ \delta$	compounds	$\frac{\Delta_{\text{vap}}H_{\text{b,exp}}}{\text{kJ}\cdot\text{mol}^{-1}}$	$\frac{\Delta_{\text{vap}}H_{\text{b,pred}}}{\text{kJ}\cdot\text{mol}^{-1}}$	D	$100\ \delta$
ethane	14.69	14.69	0.00	0.00	biphenyl	45.61	45.61	0.00	0.00
propane	19.00	17.95	1.05	5.50	butanone	31.30	27.43	3.87	12.36
butane	22.44	22.44	0.00	0.01	2-pentanone	33.44	32.92	0.52	1.54
2-methylpropane	21.30	21.57	0.27	1.27	3-pentanone	33.45	32.47	0.98	2.92
pentane	25.79	25.80	0.01	0.05	3-methyl-2-butanone	32.35	30.50	1.85	5.73
2-methylbutane	24.69	25.01	0.32	1.29	2-hexanone	36.35	37.22	0.87	2.38
2,2-dimethylpropane	22.74	25.02	2.28	10.01	3-hexanone	35.36	36.76	1.40	3.97
hexane	28.85	28.66	0.19	0.67	3,3-dimethyl-2-butanone	33.39	33.63	0.24	0.71
2-methylpentane	27.79	27.86	0.07	0.26	3-methyl-2-pentanone	34.16	34.86	0.70	2.05
3-methylpentane	28.06	28.18	0.12	0.43	4-methyl-2-pentanone	34.49	36.92	2.43	7.03
2,2-dimethylbutane	26.31	27.30	0.99	3.77	2-methyl-3-pentanone	33.84	34.09	0.25	0.73
2,3-dimethylbutane	27.38	27.31	0.07	0.24	2-heptanone	38.30	40.83	2.53	6.60
heptane	31.77	31.23	0.54	1.69	4-heptanone	36.20	37.60	1.40	3.86
2-methylhexane	30.62	30.44	0.18	0.59	2,4-dimethyl-3-pentanone	34.64	35.52	0.88	2.53
3-methylhexane	30.89	30.76	0.13	0.42	propanal	28.31	26.82	1.49	5.26
3-ethylpentane	31.12	30.83	0.29	0.92	butanal	31.50	32.54	1.04	3.30
2,2-dimethylpentane	29.23	29.88	0.65	2.22	2-methylpropanal	31.38	29.86	1.52	4.83
2,3-dimethylpentane	30.46	29.97	0.49	1.62	1-pentanal	33.64	36.66	3.02	8.97
2,4-dimethylpentane	29.55	30.14	0.59	2.00	ethanol	38.56	41.75	3.19	8.27
3,3-dimethylpentane	29.62	30.86	1.24	4.18	1-propanol	41.44	42.58	1.14	2.74
2,2,3-trimethylbutane	28.90	29.33	0.43	1.50	2-propanol	39.85	38.42	1.43	3.58
octane	34.41	33.65	0.76	2.21	1-butanol	43.29	43.67	0.38	0.87
2-methylheptane	33.26	32.85	0.41	1.22	2-butanol	40.75	39.89	0.86	2.11
3-methylheptane	33.66	33.17	0.49	1.44	2-methyl-1-propanol	41.82	43.12	1.30	3.11
4-methylheptane	33.35	33.42	0.07	0.21	2-methyl-2-propanol	39.07	36.18	2.89	7.40
3-ethylhexane	33.59	33.25	0.34	1.02	1-pentanol	44.36	44.98	0.62	1.40
2,2-dimethylhexane	32.07	32.29	0.22	0.70	2-pentanol	41.40	41.40	0.00	0.01
2,3-dimethylhexane	33.17	32.38	0.79	2.38	2-methyl-1-butanol	45.19	44.26	0.93	2.06
2,4-dimethylhexane	32.51	32.63	0.12	0.36	3-methyl-1-butanol	44.07	44.43	0.36	0.82
2,5-dimethylhexane	32.54	32.80	0.26	0.80	2-methyl-2-butanol	39.04	40.24	1.20	3.06
3,3-dimethylhexane	32.31	33.27	0.96	2.98	1-hexanol	44.50	46.45	1.95	4.37
3,4-dimethylhexane	33.24	32.95	0.29	0.88	2-hexanol	41.01	43.02	2.01	4.89
2-methyl-3-ethylpentane	32.93	32.45	0.48	1.45	2-methyl-1-pentanol	50.20	45.72	4.48	8.91
3-methyl-3-ethylpentane	32.78	32.70	0.08	0.23	3-methyl-1-pentanol	56.31	45.97	10.34	18.36
2,2,3-trimethylpentane	31.94	31.82	0.12	0.38	4-methyl-2-pentanol	44.20	42.72	1.48	3.36
2,2,4-trimethylpentane	30.79	31.99	1.20	3.91	3-methyl-3-pentanol	54.29	52.42	1.87	3.44
2,3,3-trimethylpentane	32.12	32.48	0.36	1.11	2-ethyl-1-butanol	43.20	45.80	2.60	6.01
2,3,4-trimethylpentane	32.36	32.08	0.28	0.87	1-heptanol	48.12	48.02	0.10	0.20
nonane	36.91	35.96	0.95	2.58	1-octanol	50.63	49.67	0.96	1.89
2-methyloctane	36.10	35.16	0.94	2.60	2-octanol	44.40	46.44	2.04	4.59
2,2-dimethylheptane	34.60	34.60	0.00	0.01	2-ethyl-1-hexanol	54.20	49.02	5.18	9.55
2,2,3-trimethylhexane	34.77	34.13	0.64	1.85	1-decanol	50.21	53.13	2.92	5.82
2,2,4-trimethylhexane	34.02	34.37	0.36	1.05	phenol	45.69	46.40	0.71	1.55
2,2,5-trimethylhexane	33.65	34.55	0.90	2.67	2-methylphenol	45.20	45.78	0.58	1.29
3,3-diethyl pentane	34.61	34.15	0.46	1.32	3-methylphenol	47.40	45.77	1.63	3.44
2,2,3,3-tetramethylpentane	34.30	34.23	0.07	0.22	4-methylphenol	47.50	46.41	1.09	2.30
2,2,3,4-tetramethylpentane	33.70	33.83	0.13	0.38	2,4-dimethylphenol	47.10	48.46	1.36	2.88
2,2,4,4-tetramethylpentane	38.30	36.34	1.96	5.12	2,5-dimethylphenol	46.90	49.37	2.47	5.27
2,3,3,4-tetramethylpentane	34.50	34.48	0.02	0.04	2,6-dimethylphenol	44.50	46.16	1.66	3.73
decane	38.75	38.19	0.56	1.44	3,4-dimethylphenol	49.70	48.04	1.66	3.34
2-methylnonane	38.23	37.40	0.83	2.18	3,5-dimethylphenol	49.30	46.97	2.33	4.73
3-methylnonane	38.26	37.72	0.54	1.42	diethyl ether	26.52	24.48	2.04	7.71
5-methylnonane	38.14	38.21	0.07	0.19	ethyl propyl ether	28.94	28.99	0.05	0.16
2,4-dimethyloctane	36.47	37.17	0.70	1.92	butyl methyl ether	29.55	29.67	0.12	0.39
3,3,5-trimethylheptane	36.40	37.83	1.43	3.94	*tert*-butyl methyl ether	27.94	27.00	0.94	3.35
2,2,3,3-tetramethylhexane	36.20	36.46	0.26	0.72	methyl pentyl ether	32.02	33.44	1.42	4.43
2,2,5,5-tetramethylhexane	42.40	40.12	2.28	5.38	butyl ethyl ether	31.63	32.76	1.13	3.57
undecane	41.20	40.38	0.82	2.00	dipropyl ether	31.31	32.76	1.45	4.63
dodecane	43.40	42.52	0.88	2.03	diisopropyl ether	29.10	28.08	1.02	3.50
tridecane	45.65	44.64	1.01	2.22	dibutyl ether	37.24	39.09	1.85	4.96
tetradecane	47.61	46.73	0.88	1.85	diphenyl ether	47.11	47.11	0.00	0.00
pentadecane	49.45	48.81	0.64	1.30	isobutyl formate	33.60	34.34	0.74	2.19
hexadecane	51.21	50.87	0.34	0.67	methyl acetate	30.32	27.74	2.58	8.49
heptadecane	52.89	52.92	0.03	0.06	ethyl acetate	31.94	30.08	1.86	5.82
octadecane	54.46	54.96	0.50	0.92	propyl acetate	33.92	33.30	0.62	1.83
nonadecane	56.02	56.99	0.97	1.73	isopropyl acetate	32.93	32.93	0.00	0.00
eicosane	58.49	59.02	0.53	0.90	butyl acetate	36.28	36.14	0.14	0.39
cyclopropane	20.05	20.05	0.00	0.00	isobutyl acetate	33.07	34.85	1.78	5.38
cyclobutane	24.19	24.19	0.00	0.00	pentyl acetate	38.42	38.75	0.33	0.85
cyclopentane	27.30	27.21	0.09	0.33	methyl propionate	32.24	34.76	2.52	7.83
methylcyclopentane	29.08	29.09	0.01	0.03	ethyl propionate	33.88	35.30	1.42	4.20
ethylcyclopentane	31.96	31.74	0.22	0.70	propyl propionate	35.54	37.79	2.25	6.34
propylcyclopentane	34.70	34.15	0.55	1.59	methyl butanoate	33.79	35.15	1.36	4.02
butylcyclopentane	36.16	36.45	0.29	0.81	ethyl butanoate	35.47	35.02	0.45	1.28
hexylcyclopentane	41.17	40.87	0.30	0.73	methyl isobutanoate	32.61	35.25	2.64	8.11
heptylcyclopentane	43.35	43.02	0.33	0.77	ethyl isobutanoate	35.00	34.62	0.38	1.07
octylcyclopentane	45.40	45.13	0.27	0.59	2-propenyl acetate	36.30	36.30	0.00	0.00
nonylcyclopentane	47.24	47.22	0.01	0.03	methylamine	25.60	25.60	0.00	0.00

Table 4. Continued

compounds	$\Delta_{\mathrm{vap}}H_{\mathrm{b,exp}}$ kJ·mol^{-1}	$\Delta_{\mathrm{vap}}H_{\mathrm{b,pred}}$ kJ·mol^{-1}	D	100 δ
decylcyclopentane	49.00	49.30	0.30	0.62
dodecylcyclopentane	52.59	53.41	0.82	1.55
tridecylcyclopentane	54.31	55.45	1.14	2.10
cis-1,2-dimethylcyclopentane	31.70	31.17	0.53	1.67
trans-1,2-dimethylcyclopentane	30.86	30.71	0.14	0.46
cis-1,3-dimethylcyclopentane	30.40	31.42	1.02	3.34
1,1-dimethylcyclopentane	30.29	29.17	1.13	3.72
cyclohexane	29.97	29.73	0.24	0.80
methylcyclohexane	31.27	31.34	0.07	0.21
ethylcyclohexane	34.04	33.82	0.22	0.64
propylcyclohexane	36.07	36.13	0.06	0.16
butylcyclohexane	38.49	38.36	0.13	0.35
decylcyclohexane	50.38	51.03	0.66	1.30
1,1-dimethylcyclohexane	32.51	31.25	1.26	3.88
cis-1,2-dimethylcyclohexane	33.47	33.25	0.22	0.65
trans-1,2-dimethylcyclohexane	32.96	32.80	0.16	0.49
cis-1,3-dimethylcyclohexane	32.91	33.50	0.59	1.79
trans-1,3-dimethylcyclohexane	33.39	33.05	0.34	1.03
cis-1,4-dimethylcyclohexane	33.28	33.75	0.47	1.40
trans-1,4-dimethylcyclohexane	32.56	33.29	0.73	2.25
1-butene	22.07	20.59	1.48	6.71
cis-2-butene	23.34	23.54	0.20	0.88
trans-2-butene	22.72	23.09	0.37	1.63
1-pentene	25.20	24.75	0.45	1.78
cis-2-pentene	23.34	25.32	1.98	8.50
trans-2-pentene	22.72	24.87	2.15	9.46
2-methyl-1-butene	25.50	25.47	0.03	0.11
2-methyl-2-butene	26.31	27.23	0.92	3.52
3-methyl-1-butene	24.10	24.46	0.36	1.48
1-hexene	28.30	28.15	0.15	0.54
cis-2-hexene	29.10	28.03	1.07	3.66
trans-2-hexene	28.90	27.58	1.32	4.56
cis-3-hexene	28.70	28.16	0.54	1.89
trans-3-hexene	28.90	27.70	1.20	4.14
2-methyl-1-pentene	28.10	28.37	0.27	0.97
3-methyl-1-pentene	26.90	27.93	1.03	3.81
4-methyl-1-pentene	27.10	27.85	0.75	2.76
3-methyl-*trans*-2-pentene	28.80	29.37	0.57	1.99
4-methyl-*cis*-2-pentene	29.30	27.99	1.31	4.48
4-methyl-*trans*-2-pentene	27.60	27.53	0.07	0.24
2-methyl-2-pentene	28.00	28.05	0.05	0.19
2,3-dimethyl-2-butene	29.64	27.16	2.48	8.38
1-heptene	31.10	31.12	0.02	0.06
5-methyl-1-hexene	33.85	31.07	2.78	8.22
1-octene	34.07	33.83	0.24	0.71
1-nonene	36.32	36.37	0.05	0.14
1-decene	38.66	38.79	0.13	0.33
1-undecene	40.88	41.13	0.25	0.60
1-dodecene	42.97	43.40	0.43	1.00
1-tridecene	44.98	45.62	0.64	1.43
1-tetradecene	46.90	47.81	0.91	1.93
1-pentadecene	48.66	49.97	1.30	2.68
1-hexadecene	50.42	52.10	1.68	3.33
1-octadecene	54.27	56.31	2.04	3.76
1,2-butadiene	24.27	23.62	0.65	2.67
1,3-butadiene	22.47	22.47	0.00	0.00
1,2-pentadiene	27.57	25.98	1.59	5.76
3-methyl-1,2-butadiene	27.24	29.63	2.39	8.79
benzene	30.72	31.83	1.11	3.62
methylbenzene	33.18	32.52	0.66	1.98
1,4-dimethylbenzene	35.67	36.71	1.04	2.92
1,2-dimethylbenzene	36.24	35.25	0.99	2.72
1,3-dimethylbenzene	35.66	35.66	0.00	0.00
ethylbenzene	35.57	34.51	1.06	2.99
1,2,3-trimethylbenzene	40.04	40.14	0.09	0.24
1,2,4-trimethylbenzene	39.25	41.60	2.35	5.98
1,3,5-trimethylbenzene	39.04	40.94	1.91	4.88
1,2,4,5-tetramethylbenzene	53.40	49.47	3.93	7.36
1-methyl-2-ethylbenzene	38.87	37.49	1.38	3.56
1-methyl-3-ethylbenzene	38.54	37.89	0.65	1.68
1-methyl-4-ethylbenzene	38.41	38.94	0.53	1.39
propylbenzene	38.24	37.04	1.21	3.16
isopropylbenzene	37.53	35.84	1.70	4.52
1-methyl-3-isopropylbenzene	38.12	39.45	1.34	3.51
butylbenzene	38.87	39.44	0.57	1.46
sec-butylbenzene	37.95	38.31	0.36	0.95
1,4-diethyl benzene	39.37	40.97	1.60	4.06
dimethylamine	26.40	25.60	0.80	3.02
propylamine	29.55	31.04	1.49	5.04
isopropylamine	27.83	27.69	0.14	0.51
trimethylamine	22.94	23.47	0.53	2.32
butylamine	31.81	33.31	1.50	4.72
isobutylamine	30.61	32.77	2.16	7.04
sec-butylamine	29.92	30.10	0.18	0.59
tert-butylamine	28.27	28.27	0.00	0.00
diethyl amine	29.06	30.90	1.84	6.34
pentylamine	34.01	35.43	1.42	4.16
hexylamine	36.54	37.47	0.93	2.55
triethylamine	31.01	30.09	0.92	2.96
dipropylamine	33.47	33.89	0.42	1.26
diisopropylamine	30.40	30.38	0.02	0.06
cyclohexylamine	36.14	36.14	0.00	0.00
dibutylamine	38.44	37.24	1.20	3.13
1,2-ethanediamine	41.84	39.00	2.84	6.79
1,3-propanediamine	40.85	40.48	0.37	0.90
benzenamine	41.84	41.84	0.00	0.00
2-methylbenzenamine	45.34	45.69	0.36	0.79
3-methylbenzenamine	45.61	45.68	0.07	0.15
4-methylbenzenamine	44.77	44.34	0.43	0.95
pyridine	35.09	35.53	0.44	1.25
2-methylpyridine	36.17	35.91	0.26	0.71
3-methylpyridine	37.35	37.02	0.33	0.88
4-methylpyridine	37.51	37.19	0.32	0.86
2,3-dimethylpyridine	39.08	38.70	0.38	0.97
2,5-dimethylpyridine	38.68	38.70	0.02	0.06
2,6-dimethylpyridine	37.46	37.60	0.14	0.36
3,4-dimethylpyridine	39.99	39.98	0.01	0.04
3,5-dimethylpyridine	39.46	39.81	0.35	0.89
propanenitrile	31.81	28.72	3.09	9.71
butanenitrile	33.68	36.89	3.21	9.54
2-methylpropanenitrile	32.39	32.39	0.00	0.00
pentanenitrile	36.09	41.55	5.46	15.12
decanenitrile	66.84	55.29	11.56	17.29
chloroethane	24.65	22.21	2.44	9.91
1-chloropropane	27.18	27.58	0.40	1.49
2-chloropropane	26.30	25.36	0.94	3.56
1-chlorobutane	30.39	31.49	1.10	3.62
2-chlorobutane	29.17	29.34	0.17	0.59
2-chloro-2-methylpropane	27.55	27.55	0.00	0.00
1-chloropentane	33.15	34.70	1.55	4.68
1,1-dichloroethane	28.70	29.31	0.61	2.13
bromoethane	27.04	25.00	2.04	7.53
1-bromopropane	29.84	29.70	0.14	0.46
2-bromopropane	28.33	29.00	0.67	2.35
1-bromobutane	32.51	33.19	0.68	2.08
methylthio ethane	29.50	29.09	0.41	1.39
1-methylthio propane	32.08	32.53	0.45	1.39
2-methylthio propane	30.71	30.90	0.19	0.63
1-methylthio butane	34.47	35.42	0.95	2.76
1,1,2-trichloroethane	34.82	34.21	0.61	1.76
methylthio methane	26.95	26.36	0.59	2.19
ethanethiol	26.79	24.54	2.25	8.38
1-propanethiol	29.54	29.27	0.27	0.90
2-propanethiol	27.91	27.65	0.26	0.93
1-butanethiol	32.23	32.77	0.54	1.69
2-butanethiol	30.59	31.23	0.64	2.08
2-methyl-1-propanethiol	31.01	31.98	0.97	3.13
2-methyl-2-propanethiol	28.45	28.45	0.00	0.00
1-pentanethiol	34.88	35.71	0.83	2.39
1-hexanethiol	37.20	38.35	1.15	3.10
1-heptanethiol	39.80	40.81	1.01	2.53
acetic acid	23.70	26.27	2.57	10.85
propanoic acid	32.30	37.73	3.62	10.61
acrylic acid	44.10	44.10	0.00	0.00
butanoic acid	41.80	41.00	0.80	1.91
2-methylpropanoic acid	41.13	38.92	2.21	5.38
pentanoic acid	44.10	43.78	0.32	0.72
3 methylbutanoic acid	43.20	43.24	0.04	0.08
hexanoic acid	51.10	46.31	4.79	9.38
octanoic acid	58.50	50.95	7.55	12.91
benzoic acid	50.63	50.63	0.00	0.00
1,2-dimethoxyethane	31.42	31.12	0.30	0.95
diethoxymethane	31.33	31.33	0.00	0.00

[a] D is the absolute difference. $D = |\Delta_{\mathrm{vap}}H_{\mathrm{b,exp}} - \Delta_{\mathrm{vap}}H_{\mathrm{b,pred}}|$.

in Table 2. Table 3 gives the distribution of $\bar{\delta}$ obtained for all compounds from the basic database.

$$\mathrm{AAD} = \frac{\sum |\Delta_{\mathrm{vap}}H_{\mathrm{b,exp}} - \Delta_{\mathrm{vap}}H_{\mathrm{b,pred}}|}{n} \qquad (10)$$

$$\delta = \left|\frac{\Delta_{\mathrm{vap}}H_{\mathrm{b,exp}} - \Delta_{\mathrm{vap}}H_{\mathrm{b,pred}}}{\Delta_{\mathrm{vap}}H_{\mathrm{b,exp}}}\right| \qquad (11)$$

$$\bar{\delta} = \frac{1}{N}\sum_{n}\left|\frac{\Delta_{\mathrm{vap}}H_{\mathrm{b,exp}} - \Delta_{\mathrm{vap}}H_{\mathrm{b,pred}}}{\Delta_{\mathrm{vap}}H_{\mathrm{b,exp}}}\right| \qquad (12)$$

Results presented in Table 4 denote that the predicted $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ agrees well with the experimental results. For the 311 organic compounds, Table 2 shows that the proposed method gave the best prediction results; the overall average absolute difference for $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ is 1.00 $\mathrm{kJ \cdot mol^{-1}}$, and 2.7 % is the relative deviation. More-over, the average estimation errors did not exceed 4.5 % for all of the chemical families under study.

In the case of Riedel,[7] Chen,[8] Vetere,[10] and Liu[12] methods, the correlating results were not the poorest, with the overall average absolute percentage deviations of 4.0 %, 3.8 %, 2.9 % and 3.0 %, respectively. Such methods, however, are not fully predictive, since the critical temperature, critical pressure, and/or the normal boiling point as the input parameters are absolutely needed in calculating $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$. Furthermore, it is noteworthy that these four methods all failed to correlate the $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ data of organic acid with the overall average absolute percentage deviations of 27.4 %, 35.4 %, 11.8 %, and 11.5 %, respectively.

Note, however, that Joback and Reid[19] method gave the poorest prediction results with an overall average absolute percentage deviation of 36.8 %. In general, this method is based only on the first-level group contribution and has the advantage of not requiring any input property. However, owing its oversimplification of the molecular structure, a much simpler group-contribution approach, and a relatively small data set used for estimation of group-contributions, the groups used in this model are indistinguishable between the molecular structures of isomers, which has largely limited the applicability of this approach.

Table 3 shows that, for the Joback and Reid[19] method, there are nearly 80 % of the organic compounds with $\bar{\delta} \geq 4.0$ %, while for the other methods, nearly 80 % of the organic compounds with $\bar{\delta} \leq 4.0$ % are able to be reproduced. Especially for our proposed method, there are only 2.6 % of the organic compounds with $\bar{\delta} > 10.0$ %, which further demonstrated that the proposed method is more precise and stable and has a greater range of applicability.

B. Uncertainty of this New Method. According to 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 0.9789, the F distribution value is 56.9943, and the degree of confidence is 0.9993, which further confirms the greater precision of our positional distributive contribution method for the prediction of $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$.

IV. Conclusion

The positional distributive contribution method, recently proposed for the calculation of the critical properties, is extended to the prediction of the enthalpy of vaporization at the normal boiling point. To evaluate the performance of our model, the new model has been compared with some other methods, including Riedel,[7] Chen,[8] Vetere,[10] Liu,[12] and Joback and Reid[19] methods. Contributions for compounds containing carbon, hydrogen, oxygen, nitrogen, chlorine, and sulfur were reported, and the positional distributive function has been developed which could distinguish between the thermodynamic properties of all isomers of organic compounds including *cis*- and *trans*- or *Z*- and *E*- structures. The results indicate that our method provides very satisfactory results. The overall average absolute difference for $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ predictions of the 311 organic compounds is 1.00 $\mathrm{kJ \cdot mol^{-1}}$, and 2.7 % is the relative deviation. Compared to the currently used prediction methods, the new proposed method has the advantage of not requiring any input property, is simpler to apply, is more precise and stable, and has a greater range of applicability. The higher prediction accuracy of the proposed method shown in our previous works and this work suggests that it is possible to use a totally same universal framework to predict the critical properties and the thermodynamics properties of organic compounds containing various functionalities.

Appendix A

Example 1. Prediction of $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ of ethyl isobutanoate.

This compound is decomposed in position groups as follows: 1 $\mathrm{C-(CH_2)(H)_3}$; 2 $\mathrm{C-(CH)(H)_3}$; 1 $\mathrm{C-(C)_2(CO)(H)}$; 1 $\mathrm{C-(C)(O)(H)_2}$; 1 $\mathrm{CO-(CH)(O)}$; 1 $\mathrm{O-(CO)(CH_2)}$.

The total number of groups is $N = 7$.

The position factor is the position of (CO) group: $P = 3$.

The molecular weight is $M = 116.16$.

The $\mathrm{CO-(CH)(O)}$ group and the $\mathrm{O-(CO)(CH_2)}$ group are the groups whose center is not a saturated carbon atom; therefore, N_j is 1 and 1, respectively.

From the contributions in Table 1, $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ is estimated by eq 8:

$$\Delta_{\mathrm{vap}}H_{\mathrm{b}} = 2.359 - 3.786 - 2\cdot 3.859 + 17.535 + 7.350 - 72.650\tanh(1/7) + 80.442\tanh(1/7) - 3\cdot 2.780 - 25.336\exp(1/7) + 55.293\exp(1/116.16) = 34.62\ \mathrm{kJ\cdot mol^{-1}}$$

Therefore, the calculated $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ result is 34.62 $\mathrm{kJ \cdot mol^{-1}}$, while the experimental $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ is 35.00 $\mathrm{kJ \cdot mol^{-1}}$.

Example 2. Prediction of $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ for ethylbenzene.

This compound is decomposed in position groups as follows: 5 $\mathrm{Cb-(H)}$; 1 $\mathrm{Cb-(C)}$; 1 $\mathrm{C-(Cb)(H_2)(C)}$; 1 $\mathrm{C-(H)_3(CH_2)}$.

The five $\mathrm{Cb-(H)}$ groups and the one $\mathrm{Cb-(C)}$ group are the groups whose center is not a saturated carbon atom; therefore, N_j is 5 and 1, respectively.

The total number of groups is $N = 8$.

The molecular weight is $M = 106.17$.

From the contributions in Table 1, $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ is estimated by eq 8:

$$\Delta_{\mathrm{vap}}H_{\mathrm{b}} = 2.359 + 10.454 - 3.786 + 4.46\tanh(5/8) - 32.99\tanh(1/8) - 25.335\exp(1/8) + 55.293\exp(1/106.17) = 34.51\ \mathrm{kJ\cdot mol^{-1}}$$

Therefore, the calculated $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ result is 34.51 $\mathrm{kJ \cdot mol^{-1}}$, while the experimental $\Delta_{\mathrm{vap}}H_{\mathrm{b}}$ is 35.57 $\mathrm{kJ \cdot mol^{-1}}$.

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