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A Group Contribution Model for Determining the Vaporization Enthalpy of Organic Compounds at the Standard Reference Temperature of 298 K

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Abstract — The vaporization enthalpy is regarded as a measure of molecular interactions in the vapor/liquid phase. It has a number of applications in chemical and petrochemical processes in which vapor-liquid equilibrium exists. Acree and Chickos [1], recently published a comprehensive compilation of phase change enthalpies, including vaporization enthalpies of pure organic and organometallic compounds. This collection of vaporization enthalpies for 2811 compounds at the standard temperature of 298.15 K was used in this study for the development of a predictive model. The compounds in the collection are composed of a combination of the following atoms, viz. carbon, hydrogen, nitrogen, oxygen, phosphorous, sulfur, fluorine, chlorine, bromine, and iodine. This paper presents a reliable group contribution model for the prediction of the vaporization enthalpies of organic compounds. The group contribution model developed is able to predict the standard molar enthalpies of vaporization to within an average absolute relative deviation of 3.7%, which is of sufficient accuracy for many practical applications in chemical and petrochemical engineering.

Keywords: Vaporization enthalpy, Group Contribution, Organic Compounds; Chemical Structure, Reliable model.

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1. Introduction

The vaporization enthalpy is the difference between the enthalpies of a unit mole of the saturated vapor and the saturated liquid of a compound [2]. Therefore, it may be considered as a measure of the strength of intermolecular forces in the liquid/vapor phase.

The vaporization enthalpy along with vapor pressure is regarded as one of the fundamental properties needed in the design and the optimization of various chemical and petrochemical processes in which vapor-liquid phase change occurs. Furthermore, it is regarded as one of the basic properties used to predict other physico-chemical properties.

The estimation of the vaporization enthalpy at a standard temperature of 298.15 K has been the subject of many studies. Depending on the type of input parameters used, all the correlations proposed to date can be categorized into three major classes.

The first category includes those correlations which relate the vaporization enthalpy to the other physical properties, i.e. normal boiling temperature, critical properties, acentric factor, and vapor pressure. The correlations proposed by Fishtine [3-5], Wadsö [6], and Zhao et al. [7, 8] originate from Trouton's rule [9] which uses the normal boiling temperature to estimate the vaporization enthalpy. The Clapeyron [2], Antoine [2], Reidel [10], Wagner [11, 12], and Ambrose–Walton [13] equations use vapor pressure and critical properties to estimate the vaporization enthalpy. The correlations proposed by Pitzer [14], Wang–Shi [15], and Morgan–Kobayashi [16] are based on corresponding states principle which uses critical properties and the acentric factor to correlate the vaporization enthalpy. The models proposed by Giacalone [2], Kistiakowsky [2], Chen [17], Vetere [18, 19], and Liu [20] relate the vaporization enthalpy to vapor pressure and the normal boiling temperature.

The second category comprises those correlations which use just the chemical structure-based parameters. Several quantitative-structure property relationships have so far been proposed by Ren [21], Zhokhova et al. [22], and Krasnykh et al. [23]. Lin et al. [24] and Wang et al. [25] used the solvation free energy to correlate the vaporization enthalpy. Another chemical structure-based approach that have been widely considered by various research groups to correlate the vaporization enthalpy is that of group contribution [26-46]. Chen [47] used the quasi-chemical lattice theory-based approach to predict the vaporization enthalpy. Stefanis et al. [48] proposed a group contribution model based on the theory of non-random hydrogen bonding equation of state.

The third category includes those correlations in which both the chemical structure-based parameters and the physical properties are used to predict the vaporization enthalpy. Screttas and Micha-Screttas [49] employed the normal boiling temperature and carbon number to estimate the vaporization enthalpy of homologous series of compounds. Greenshields and Rossini [50] correlated the vaporization enthalpy with the normal boiling temperature and some parameters taking into account chain branching. There are several group contribution-based models which use other physical properties to estimate the vaporization enthalpy [51-59].

It should be noted that correlations that have been proposed for normal boiling temperature vaporization enthalpy [60-63] have not been reviewed in this study.

The correlations within the first and third group suffer from a general shortcoming. As mentioned earlier, they relate the vaporization enthalpy to other physical properties. It means that they cannot produce an estimation when the required physical properties are not available. From this point of view, the second category of correlaions, viz. the methods which use just chemical structure-based parameters, surpasses the other two categories. Another point that needs to be considered is that the majority of the correlations proposed to date for the estimation of the vaporization enthalpy have been developed and evaluated using a relatively small number of experimental data. As a result, there are some limitations in their applications.

Recently, Acree and Chickos [1] reviewed the literature for published phase change enthalpies at the standard temperature of 298.15 K over the period 1880-2010 and presented their results in an enormous compilation. The main aim of this study is to develop a group contribution method using this large database.

2. Experimental enthalpy of vaporization database

The data compilation collected by Acree and Chickos [1] was used to provided the main database of vaporization enthalpy at the standard temperature of 298.15 K. The data compilation was supplemented with recently published enthalpies of vaporization taken from the chemical literature [64-156].

The database consists of 4320 experimental data points for 2811 compounds. Single experimental values were reported for 2049 compounds. Multiple experimental values were reported for the remaining 762 compounds, with the arithmetic average being used where multiple value exist. It should be noted that no attempt was made to choose between the independently determined values, which for the most part differed by less than 9 $kJ.mol^{-1}$. The exceptions to this are presented in Table 1.

Table 1

A thorough component analysis of the compounds within the dataset demonstrates that the vaporization enthalpy enthalpies range between 15.6 and 424.5 $kJ.mole^{-1}$. The compounds are composed of carbon (1 to 92 atoms per compound), hydrogen (1 to 186 atoms per compound), nitrogen (1 to 5 atoms per compound), oxygen (1 to 10 atoms per compound), phosphorus (1 to 2 atoms per compound), sulfur (1 to 3 atoms per compound), fluorine (1 to 50 atoms per compound), chlorine (1 to 10 atoms per compound), bromine (1 to 3 atoms per compound), and iodine (1 to 2 atoms per compound). There are 689 hydrocarbons (C and H compounds) in the dataset whose vaporization enthalpies range from 20.1 to 424.5 $kJ.mole^{-1}$. The data set includes 503 nitrogen compounds whose vaporization enthalpies range from 25.2 to 121.5 $kJ.mole^{-1}$. The elemental composition analysis of the dataset further shows that there are 1424 oxygenated compounds whose vaporization enthalpies range from 15.6 to 236.2 $kJ.mole^{-1}$. There are 162 sulfur compounds in the dataset having vaporization enthalpies that range from 23.8 to121.5 $kJ.mole^{-1}$. There are a significant number of halogenated compounds within the dataset: 204 fluorine-containing compounds with vaporization enthalpies between 15.6 and 141 kJ mol^{-1}; 211 chlorine-containing compounds with vaporization enthalpies between 20 and 120.2 kJ mol^{-1}; 54 bromine-containing compounds having vaporization enthalpies that range between 23.8 and 96.1 $kJ.mole^{-1}$; and 33 iodine-containing compounds whose vaporization enthalpies range between 31.8 and 118.5 $kJ.mole^{-1}$. There are 40 phosphorous-containing compounds in the dataset that have vaporization enthalpies ranging between 29.1 and 104.5 $kJ.mole^{-1}$. The chemical diversity of the dataset considered in the present study is significantly greater than datasets used in earlier studies [46] involving the prediction of vaporization enthalpies.

In order to develop a predictive model the K-means clustering technique [157, 158] was used to portion the main database into three sub-groups, viz. the training, the validation, and the test sets. The training set (comprising 2249 compounds) was used to develop the model. Next, the validation set (comprising 281 compounds) was used to evaluate the the validity of the model developed. Finally, the test set (containing the remaining 281 compounds) was used to assess the predictive capability of the model.

3. Model development

The physio-chemical properties of chemical compounds may be regarded as the intermolecular interactions originating from their chemical sub-structures. Therefore, it seems to be rational that one relates the properties to an efficient subset of these chemical sub-structures. The term "efficient" means a subset which enables one to distinguish each chemical compound from the others. In order to find an efficient subset of chemical sub-structures to predict the vaporization enthalpy, 1600 chemical sub-structures which have been previously used by the authors to correlate other important properties [159-163] were generated. Next, the number of occurrences of each of these 1600 chemical sub-structures in chemical structures of the chemical compounds were collected in a table. Then, the pair correlation between each pair of these 1600 chemical substructures was considered as the major criteria to prevent entering irrelevant chemical sub-structures. In this step, if the pair correlation of a pair was more than the threshold value of 0.95, one of them was eliminated and the other kept for the subsequent computations. Following these preliminary calculations, the collection of chemical structures was reduced to 323 chemical sub-strutures.

In order to find the optimal subset of chemical sub-structures affecting the vaporization enthalpy and also to develop the final model, the sequential search forward selection method was implemented [160]. A flowchart for the algorithm is shown in Figure 1.

Figure 1

The algorithm starts by evaluating one-chemical sub-structure linear correlations. The first optimal chemical-substructure is the one whose correlation produces the lowest average absolute relative deviation (%AARD) from experimental data. In the next step, the algorthim considers the subset of two-chemical sub-structures of which one of them is the first optimal chemical sub-struture selected in the previous step. The optimal subset of two chemical sub-structures is the one represents the experimental data with the lowest possible %AARD. This process is followed by the algorithm by gradual increasing the number of chemical sub-structures to achieve a desired improvement in the value of %AARD. In this study, the stopping criterion is set at a 0.01 improvement in the %AARD value. It means that the algorithm was set to stop if the improvement in %AARD was lower than 0.01%. The statistical parameters used in this study are defined in Appendix A.

4. Result and discussion

The procedure outlined in the previous section was pursued by introducing the collection of 323 chemical sub-structures into the sequential seach forward selection algorithm.

According to the algorithm, the optimal vaporization enthalpy model includes 150 chemical sub-strutures. The model obtained is as follows:

$$\Delta_{vaporization}H_m{}^{\circ}(kJ.mol^{-1}) = \sum_{i=1}^{150} n_i \times \Delta_{vaporization}H_m{}^{i} + \Delta_{vaporization}H_m{}^{0} \tag{2}$$

where $\Delta_{vaporization}H_m{}^{0}$, $\Delta_{vaporization}H_m{}^{i}$ and n_i are the intercept of the equation, the contribution of the *i*th chemical sub-structure to the vaporization enthalpy and the number of occurrences of the *i*th chemical sub-structure in every chemical structure of pure compounds, respectively. The subset of 150 chemical sub-structures and their contribution to the vaporization enthalpy are tabulated in Table 2.

Table 2

The predicted vaporization enthalpies and their %AARD from the experimental values are presented as a supplementary table.

The model results demonstrate that it can successfully predict the standard molar vaporization enthalpies of pure organic compounds at 298 K. The %AARD, standard deviation error, and root mean square error of calculated values based on the model from the experimentally measured vaporization enthalpies are 3.7%, 4.45, and 4.45 for the training set, 3.7%, 4.51, and 4.52 for the validation set, and 3.7%, 3.78, and 3.78 for the test set, respectively.

In order to present the applicability domain of the model and detect the outliers of the model, a Williams [164] plot is presented in Figure 2.

Figure 2

In this plot, the hat values and the standardized results are implemented (presented in a supplementary table). In this plot, a warning leverage ($h^*=0.35$) - blue vertical line – is generally fixed at 3p/n, where p is the number of model variables plus one and n is the number of training chemicals. The leverage of 3 is regarded as a cut-off value to approve the points that lie ± 3 (two horizontal red lines) standard deviations from the mean (to cover 99% normally distributed data). The applicability domain is the region of $0 \leq h \leq 0.35$ and $-3 \leq R \leq +3$. As depicted in Figure 2, the majority of the data points lie in this domain which indicates the validity of both the model development and validation. The data points shown with red circles ($3<R$ or $R<-3$) are "bad high leverage" points and represent outliers of the model. This erroneous prediction could probably be attributed to incorrect experimental data rather than to the molecular structure [164].

According to the Wiliams plot, there are 71 outliers in the database. The outliers and their chemical structures are presented in a supplementary table.

The elemental analysis of the model results are presented in Table 3.

Table 3

According to the results, the model predicts the enthalpies of 689 hydrocarbons with an *%AARD* of 2.4%. There are 14 hydrocarbons for which the model shows an *%AARD* of more than 10%. The compounds are trans 2,2,4,6,6-pentamethyl-3-heptene (24%), cis 2,2,4,6,6-pentamethyl-3-heptene (20.7%), cis 1,2-diphenylethylene (20.3%), 4,4-dimethyl-1-hexene (19.5%), 1-cyclopropyl-1,3-pentadiene (19.2%), 1-trans-5-trans-9-cis-cyclododecatriene (13.8%), 1,1,4-trimethylcyclohexane (12%), bicyclo[2.2.1]hepta-2,5-diene (11.7%), dibenz[a,c]anthracene (10.9%), 5,5-bis(3,3’-dimethylbutyl)-2,2,8,8-tetramethylnonane (10.5%), 5-ethylidene-2-norbornene (10.4%), perylene (10.3%), and 2-methylbicyclo[2.2.2]oct-2-ene (10%). Figure S1 (please see supplementary file) shows the estimated vaporization enthalpies of hydrocarbons versus the corresponding experimental values.

The model predictions for nitrogen compounds versus the corresponding experimental vaporization enthalpies are shown in Figure S2 (please see supplementary file). As shown, the *%AARD* of the model from experimental data is 4.7%. According to the Williams plot shown in Figure 2, 15 out of the 71 outliers of the model are for nitrogen compounds.

The *%AARD* of the model results from experimental vaporization enthalpy for oxygenated compounds is 4.5%. The predicted values versus the corresponding experimental data are shown in Figure S3 (please see supplementary file). The majority of the outliers are for oxygenated compounds (55 out of 71). Therefore, their experimental data may be erroneous. This point affects the quality of the model in the prediction of the vaporization enthalpies of the compounds. The model predicts the vaporization enthalpies of 181 of 1424 oxygenated compounds with a higher than 10% %ARD.

According to the results, the model can predict the vaporization enthalpies of the phosphorous-containing compounds with a reasonable %AARD of 2.7%. The predicted versus experimental vaporization are shown in Figure S4 (please see supplementary file).

Sulfur-containing compounds are a class of compounds for which the model shows an %*AARD* of 3.6%. There are 10 out of the 162 sulfur compounds for which the model gives an *ARD%* of higher than 10%. The compounds are benzenethiol (30.7%), trithiocarbonic acid, cyclic ethylene ester (29.5%), (dl) malathion (28.8%), divinyl sulfide (21.2%), 2-(5H)-thiophenone (18.8%), diethyl sulfite (16.7%), (ethaneperoxoato) pentafluoro sulfur (14.9%), butyl sulfonyl chloride (12.7%), O,O-diethyl-S-[2-(ethylthio)ethyl] thiophosphate (11.9%), and 4-methylthiazole (10.5%). The predicted versus experimental vaporization are shown in Figure S5 (please see supplementary file).

Fluorine-containing compounds are one of the important classes of compounds whose vaporization enthalpies are estimated by the model with an *AARD%* of 4.4%. Their predicted versus experimental vaporization data are shown in Figure S6 (please see supplementary file).

The model predicts the vaporization enthalpies of chlorine-containing compounds better than fluorine-containing compounds in terms of AARD% (3.7% vs. 4.4%). Their predicted versus experimental vaporization data are shown in Figure S7 (please see supplementary file).

Based on the model analysis, the vaporization enthalpies of bromine-containing compounds are successfully predicted by the model. The model AARD% for this class of compounds is 2.5%, which is less than those of previously mentioned halogenated compounds. Figure S8 (please see supplementary file) showss the predicted vaporization enthalpies of bromine-containing compounds versus their corresponding experimental values.

The model shows a promising %AARD of 1.8% for iodine-containing compounds. Iodine-containing compounds are another class of halogenated compounds whose vaporization enthalpies are successfully predicted by the model. Figure S9 (please see supplementary file) showss the estimated vaporization enthalpies of iodine-containing compounds versus their corresponding experimental values.

It should be mentioned that the red circles and blue stars represent the vaporization enthalpy and the relative deviation of the model results from experimental data, respectively. The red circiles should be read from the left axis and the blue stars should be read from the right axis.

Unfortunately, a comprehensive comparison between the model proposed in this sudy and previously proposed models is not possible because they have mostly been developed for small groups/classes of compounds and it is not possible to use most of the previous models for the compounds used in this study.

Very recently, Santos and Leal [46] reviewed various models for the estimation of the vaporization enthalpy at the standard temperature of 298.15. They used a dataset of 83 hydrocarbons including alkanes, alkenes, polyenes, diynes, cycloalkanes, alkylidenecycloalkenes, cycloalkenes, and benzene related compounds to compare their model with the models proposed by Ducros et al. [32, 33], Guthrie and Taylor [36], Chickos et al. [28], Domalski and Hearing [165] , Constantinou and Gani [29], and Kolská et al. [37]. We used the same dataset to compare our model with the previous models, even the one proposed by Santos and Leal [46]. The results are presented in Table 4.

Table 4

As demonstrated, the model proposed in this study predicts the vaporization enthalpies of the compounds with an %AARD of 3.1%. However, the models proposed by Ducros et al. [32, 33], Guthrie and Taylor [36], Chickos et al. [28], Domalski and Hearing [165] , Constantinou and Gani [29], and Kolská et al. [37] predicts the dataset with an %AARD of 7%, 10.6%, 4.6%, 6.4%, 5.5%, 4.1% respectively. Therfore, the model predict the vaporization enthalpies of the selected 83 compounds better than these previous models. It should be noted that the model proposed by Santos and Leal [46] estimates the vaporization enthalpies of the selected 83 hydrocarbons with an %AARD of 2.6% which shows that their model is slightly better than the present model (2.6% vs. 3.1%). However, the model proposed by Santos and Leal [46] is capable of use for just hydrocarbons, i.e. it cannot be considered as a general model. As result, the model proposed in this study can be considered better than previous models.

4. Conclusions

In this study, an extensive database of 2249 pure organic compounds (training set) was used to develop a comprehensive group contribution model for the estimation of the standard molar vaporization enthalpy of pure organic compounds at the standard temperature of 298.15 K. The model demonstrated an acceptable %AARD of 3.7% from experimental data. Next, the validity of the model was evaluated using a validation set comprised of the vaporization enthalpies of 281 pure organic compounds. The model showed the same %AARD value for the validation set (3.7%). The predictive capability of the model was assessed using the vaporization enthalpies of a test set of 281 pure organic compounds. Like the training set and the validation set, the test set was predicted by the model with an %AARD of 3.7% from the experimental values. In order to compare the model with the most-widely used methods proposed by Ducros et al. [32, 33], Guthrie and Taylor [36], Chickos et al. [28], Domalski and Hearing [165], Constantinou and Gani [29], Kolská et al. [37], and Santos and Leal [46], an external dataset of 83 hydrocarbons, previously used, by Santos and Leal [46] was also used. The results reveal that the model proposed in this study is better than previous models and it predicts the vaporization enthalpies of hydrocarbons with approximately the same accuracy of the model proposed by Santos and Leal [46].

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Appendix A

The mathematical definition of the relative deviation (%RD), average absolute relative deviation (%AARD), root mean square error (RMSE), standard deviation error (Std), and squared correlation coefficient (R^2) are presented as follows:

$$\%RD = 100 \times \frac{pred - lit}{lit} \tag{A1}$$

$$\%AARD = \frac{100}{N} \sum_{i}^{N} \frac{|pred(i) - lit(i)|}{lit(i)} \tag{A2}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} (pred(i) - lit(i))^2}{N}} \tag{A3}$$

$$Std = \frac{1}{\mathrm{N}} \sum_{i}^{\mathrm{N}} \sqrt{\left(\mathrm{pred(i)} - \overline{\mathrm{pred}}\right)^2} \tag{A4}$$

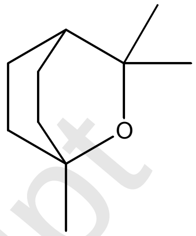
$$R^2 = 1 - \frac{\sum_{i}^{N} (pred(i) - lit(i))^2}{\sum_{i}^{N} (pred(i) - \overline{lit})^2} \tag{A5}$$

$$AE = \frac{1}{N}\sum_{i}^{N} \left| pred\,(i) - lit\,(i) \right| \tag{A6}$$

where *pred* and *lit* denote the predicted value by model and its corresponding value reported by literature, respectively. The terms $\overline{\mathrm{pred}}$ and $\overline{lit}$ refer to the mean values over the predicted values by the model and the mean value over the literature reported data. *N* is the number of data point in each data set or subset.

Appendix B

1,3,3-trimethyl-2-oxabicyclo[2.2.2]octane (1,8-cineole)



Experimental values: 51.1 kJ.mole^{-1} (average value of two reported data)

Predicted value: 49.3 kJ.mole^{-1} (3.6% deviation)

ID	$\Delta_{vaporization}H_m^i$	n_i	***value***	n_i x $\Delta_{vaporization}H_m^i$
1	$\Delta_{vaporization}H_m^0$		8.303447643	8.303447643
2	$\Delta_{vaporization}H_m^1$	3	-2.37120975	-7.11362925
4	$\Delta_{vaporization}H_m^3$	4	-0.539008082	-2.156032327
5	$\Delta_{vaporization}H_m^4$	3	-1.500466375	-4.501399124
38	$\Delta_{vaporization}H_m^{37}$	4	0.275614093	1.102456372
39	$\Delta_{vaporization}H_m^{38}$	1	1.34413169	1.34413169
51	$\Delta_{vaporization}H_m^{50}$	4	0.083209717	0.332838869
54	$\Delta_{vaporization}H_m^{53}$	14	-0.002639367	-0.036951144
73	$\Delta_{vaporization}H_m^{72}$	1	-0.515369603	-0.515369603
79	$\Delta_{vaporization}H_m^{78}$	1	3.183965622	3.183965622
87	$\Delta_{vaporization}H_m^{86}$	1	1.16437248	1.16437248
107	$\Delta_{vaporization}H_m^{106}$	10	4.340272799	43.40272799
109	$\Delta_{vaporization}H_m^{108}$	2	2.860264925	5.72052985
117	$\Delta_{vaporization}H_m^{116}$	6	-0.178616401	-1.071698406
123	$\Delta_{vaporization}H_m^{122}$	14	0.251900624	3.526608738
124	$\Delta_{vaporization}H_m^{123}$	2	-0.622053359	-1.244106717
133	$\Delta_{vaporization}H_m^{132}$	7	-0.309578657	-2.167050598
	Total			49.3

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Figure Captions

Figure 1- The flow chart of the sequential search forward selection used to select the optimal subset of chemical sub-structures.

Figure 2- Williams plot – red circles shows the outliers of the model for which the experimental values may be erroneous.

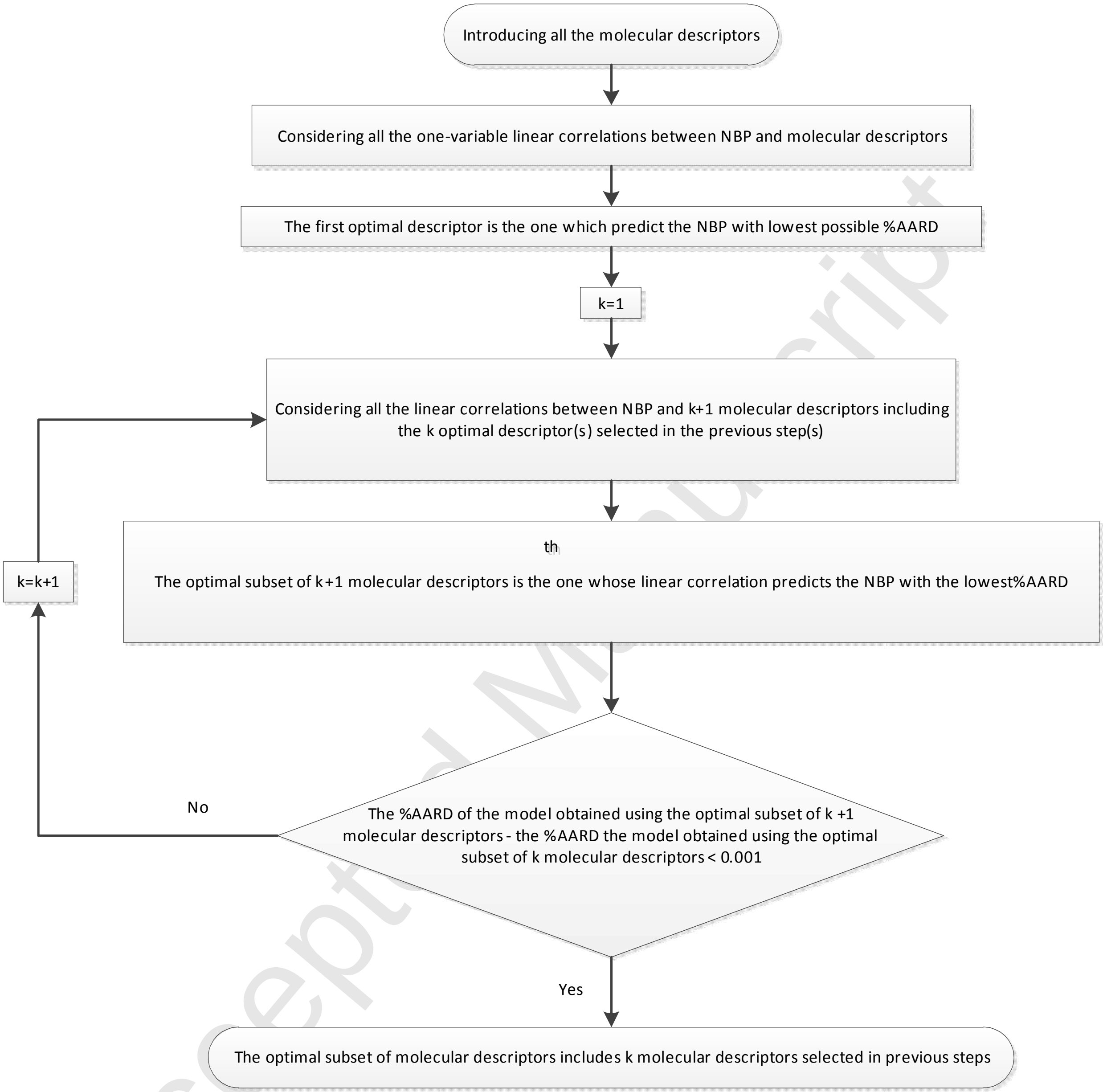

Introducing all the molecular descriptors
Considering all the one-variable linear correlations between NBP and molecular descriptors
The first optimal descriptor is the one which predict the NBP with lowest possible %AARD
k=1
Considering all the linear correlations between NBP and k+1 molecular descriptors including the k optimal descriptor(s) selected in the previous step(s)
th
The optimal subset of k+1 molecular descriptors is the one whose linear correlation predicts the NBP with the lowest%AARD
k=k+1
No
The %AARD of the model obtained using the optimal subset of k +1 molecular descriptors - the %AARD the model obtained using the optimal subset of k molecular descriptors < 0.001
Yes
The optimal subset of molecular descriptors includes k molecular descriptors selected in previous steps

Figure 1.

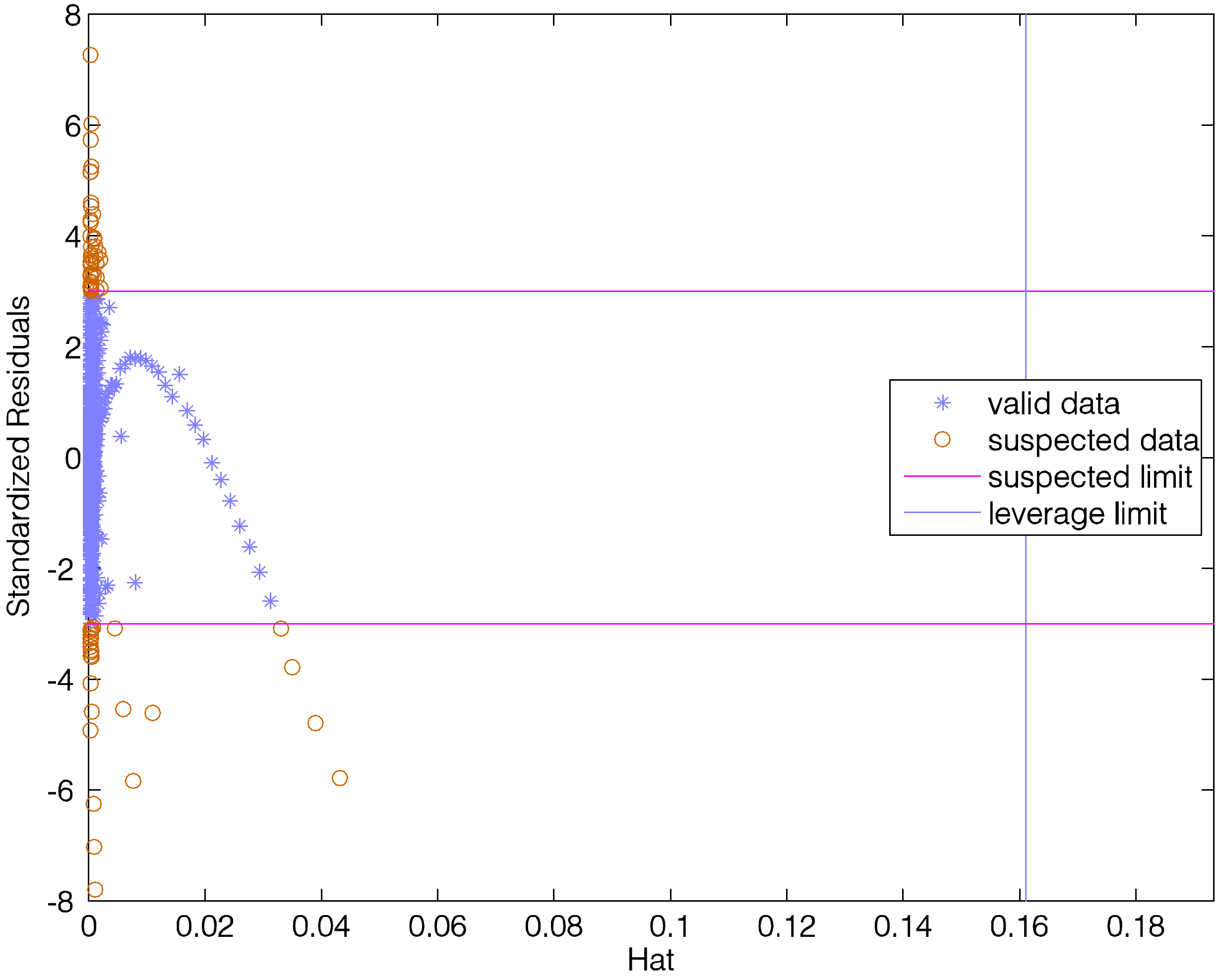

8
6
4
2
0
-2
-4
-6
-8
Standardized Residuals
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
Hat
valid data
suspected data
suspected limit
leverage limit

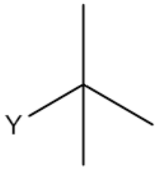
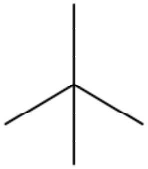
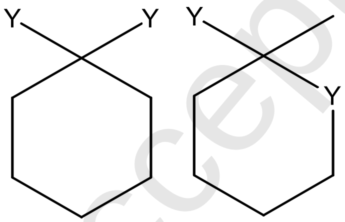
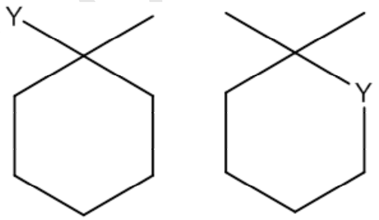
Figure 2.

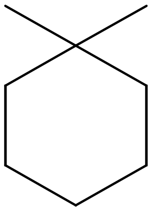
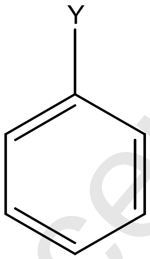
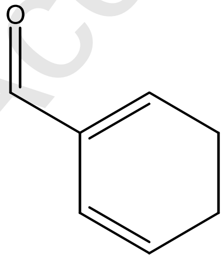
Table 1- The componds whose experimental vaporization enthalpies show more than 9 kJ.mole^{-1} in the literature

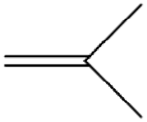
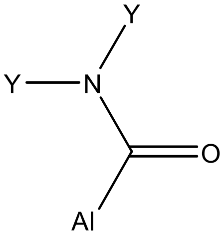
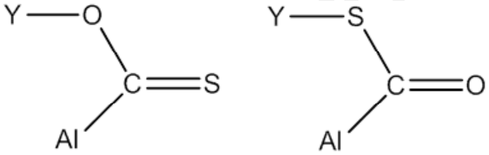
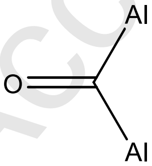
No.	Compound	$\Delta_{vaporization}H_{m}^{o\ exp}$ range/kJ.mole^{-1}			N*
1	tributyrin	84.9	-	107.1	4
2	cis 1,2-diphenylethylene (cis stilbene)	50.3	-	70.5	2
3	1,2,4-triazolo[1,5-a]pyrimidine	63.7	-	82.5	3
4	1-methylimidazole	47.2	-	64.7	7
5	pyrimidine	41	-	58.3	4
6	5-nonanone	40.2	-	55	4
7	dibutyl sulfide	40.3	-	54.2	3
8	1,2-propanediol (propylene glycol)	62.2	-	76	6
9	triethylenetetramine	71	-	84.7	3
10	benzo[e]pyrene	105	-	118.2	2
11	1,10-decanediol	113.7	-	126.6	3
12	benzo[a]pyrene	105	-	117.8	2
13	benzo[b]fluoranthene	104	-	116.8	2
14	ethylenediamine	41.6	-	54.4	6
15	triacontane	152.3	-	164.5	2
16	benzo[k]fluoranthene	105.5	-	117.4	2
17	formamide	59.5	-	70.8	7
18	hexadecane	70.6	-	81.8	10
19	N-(2-hydroxyethyl)ethylenediamine	64.2	-	75.1	2
20	octacosane	141.9	-	152.4	4
21	1-phenylimidazole	74.3	-	84.6	2
22	butyl formate	32.1	-	42.4	8
23	4-chloroaniline	52.2	-	62.3	2
24	propylene carbonate	61.3	-	71.3	4
25	diethyl oxalate	55.3	-	65.2	5
26	linalool	55.3	-	65	2
27	diisopropyl disulfide	39.6	-	49.3	2
28	benz[a]anthracene	96.6	-	105.8	2
29	benzyl alcohol	60.3	-	69.5	8
30	chrysene (benzo[a]phenanthrene)	97	-	106.2	2

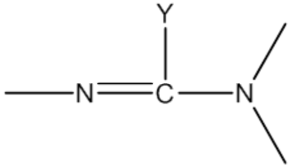
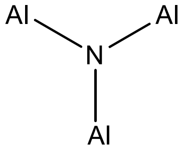
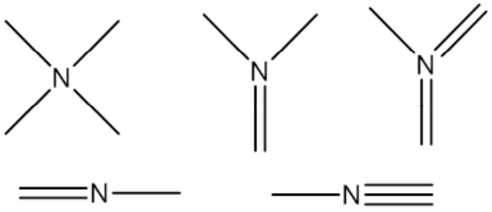
*N is the number of reported experimental data in the literature

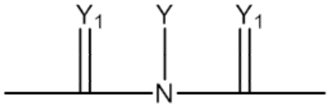
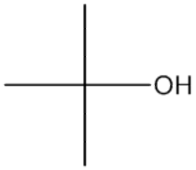
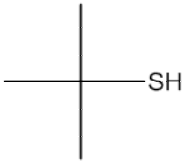
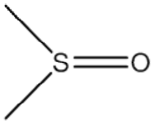
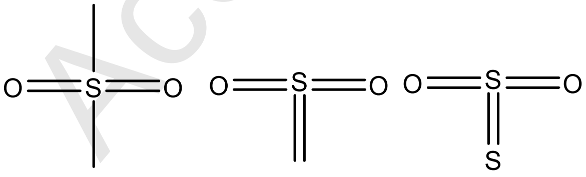
Table 2- The contribution of each chemical substructure to the vaporization enthalpy of organic compounds (parameters of eq. (2)).

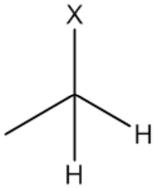
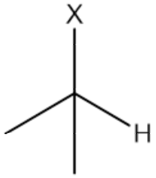
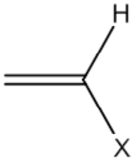
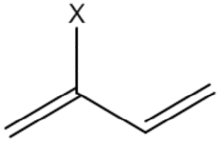
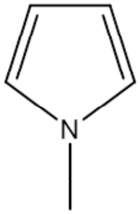
ID	$\mathbf{\Delta_{vaporization}H_m^{\,i}}$	**Chemical structure**	**Comment**	**Value**
	$\Delta_{vaporization}H_m^{\,0}$			8.303448
1	$\Delta_{vaporization}H_m^{\,1}$		number of total tertiary C(sp^3) Y = H or any heteroatom	-2.37121
2	$\Delta_{vaporization}H_m^{\,2}$		number of total quaternary C(sp^3)	0.606346
3	$\Delta_{vaporization}H_m^{\,3}$		number of ring secondary C(sp^3) Y = H or any heteroatom	-0.53901
4	$\Delta_{vaporization}H_m^{\,4}$		number of ring tertiary C(sp^3) Y = H or any heteroatom	-1.50047

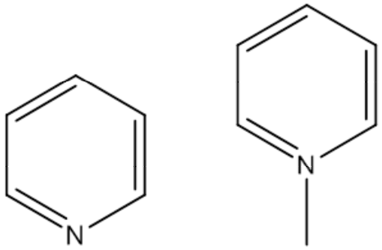
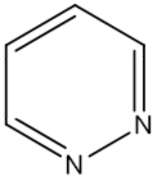
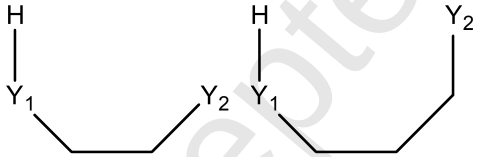
5	$\Delta_{vaporization}H_m^{5}$		number of ring quaternary C(sp^3)	-3.00716
6	$\Delta_{vaporization}H_m^{6}$	Sum of all the carbons belonging to any aromatic and heteroaromatic structure	number of aromatic C(sp^2)	-0.23441
7	$\Delta_{vaporization}H_m^{7}$		number of substituted benzene C(sp^2) Y = carbon or any heteroatom	0.37322
8	$\Delta_{vaporization}H_m^{8}$		number of non-aromatic conjugated C(sp^2)	0.445756

9	$\Delta_{\text{vaporization}}H_m{}^{9}$		number of aliphatic tertiary C(sp^2)	-0.19655
10	$\Delta_{\text{vaporization}}H_m{}^{10}$	Ar-COOH	number of carboxylic acids (aromatic)	4.297641
11	$\Delta_{\text{vaporization}}H_m{}^{11}$		number of tertiary amides (aliphatic) Y = Ar or Al (not H, not C = O) Al = H or aliphatic group linked through C	-7.74116
12	$\Delta_{\text{vaporization}}H_m{}^{12}$		number of thioesters (aliphatic) Y = Ar or Al (not H) Al = H or aliphatic group linked through C	-5.79294
13	$\Delta_{\text{vaporization}}H_m{}^{13}$		number of ketones (aliphatic)	-1.08661

14	$\Delta_{vaporization}H_m{}^{14}$		number of amidine derivatives Y = C or H	10.54162
15	$\Delta_{vaporization}H_m{}^{15}$	Al-NH$_2$	number of primary amines (aliphatic) Al = aliphatic group linked through C (not C = O)	-14.3048
16	$\Delta_{vaporization}H_m{}^{16}$		number of tertiary amines (aliphatic) Al = aliphatic group linked through C (not C = O)	-8.6937
17	$\Delta_{vaporization}H_m{}^{17}$	N#C-Al	number of nitriles (aliphatic)	12.7156
18	$\Delta_{vaporization}H_m{}^{18}$	Ar-CN	number of nitriles (aromatic)	9.570331
19	$\Delta_{vaporization}H_m{}^{19}$		number of positive charged N	3.67026

20	$\Delta_{vaporization}H_m^{20}$		number of imides (thio-) Y = H or C Y_1 = O or S	-11.6346
21	$\Delta_{vaporization}H_m^{21}$	Al-OH	number of hydroxyl groups Al = aliphatic group linked through any atom	8.848529
22	$\Delta_{vaporization}H_m^{22}$		number of secondary alcohols	1.417441
23	$\Delta_{vaporization}H_m^{23}$	Ar-O-Y	number of ethers (aromatic) Y = Ar or Al (not C = O, not C # N)	3.46586
24	$\Delta_{vaporization}H_m^{24}$		number of thiols	-16.3948
25	$\Delta_{vaporization}H_m^{25}$		number of sulfoxides	22.75399
26	$\Delta_{vaporization}H_m^{26}$		number of sulfones	24.32781

27	$\Delta_{\mathrm{vaporization}}H_m^{27}$			0.786645
28	$\Delta_{\mathrm{vaporization}}H_m^{28}$			0.376854
29	$\Delta_{\mathrm{vaporization}}H_m^{29}$			3.593147
30	$\Delta_{\mathrm{vaporization}}H_m^{30}$		number of X on exo-conjugated C	-2.12488
31	$\Delta_{\mathrm{vaporization}}H_m^{31}$		number of Oxiranes	3.820174
32	$\Delta_{\mathrm{vaporization}}H_m^{32}$		number of Pyrroles	-9.81251

33	$\Delta_{vaporization}H_m{}^{33}$		number of Pyridines	2.437621
34	$\Delta_{vaporization}H_m{}^{34}$		number of Pyridazines	15.84923
35	$\Delta_{vaporization}H_m{}^{35}$	Sum of the hydrogens linked to all of the Os and Ns in the molecule	number of donor atoms for H-bonds (N and O)	6.500187
36	$\Delta_{vaporization}H_m{}^{36}$		number of intramolecular H-bonds Y_1 = B, N, O, Al, P, S Y_2 = N, O, F The geometric distance between H and Y_2 must be in the range 1 - 2.	-3.0317
37	$\Delta_{vaporization}H_m{}^{37}$	CH_2R_2		0.275614

38	$\Delta_{vaporization}H_m{}^{38}$	CHR_3	1.344132
39	$\Delta_{vaporization}H_m{}^{39}$	CR_4	-3.5672
40	$\Delta_{vaporization}H_m{}^{40}$	CH_3X	3.02016
41	$\Delta_{vaporization}H_m{}^{41}$	CH_2RX	2.076907
42	$\Delta_{vaporization}H_m{}^{42}$	CH_2X_2	2.829842
43	$\Delta_{vaporization}H_m{}^{43}$	CHR_2X	-0.02118
44	$\Delta_{vaporization}H_m{}^{44}$	$CHRX_2$	4.442286
45	$\Delta_{vaporization}H_m{}^{45}$	$=CH_2$	-0.31895
46	$\Delta_{vaporization}H_m{}^{46}$	#CR or R=C=R	2.46037
47	$\Delta_{vaporization}H_m{}^{47}$	R--CX--X	-1.94169
48	$\Delta_{vaporization}H_m{}^{48}$	Al-CH=X	-4.92407
49	$\Delta_{vaporization}H_m{}^{49}$	X--CR..X	-1.88908
50	$\Delta_{vaporization}H_m{}^{50}$	H^a attached to $C^0(sp^3)$ no X attached to next C	0.08321
51	$\Delta_{vaporization}H_m{}^{51}$	H^a attached to $C^3(sp^3)$ or $C^2(sp^3)$ or $C^3(sp_2)$ or $C^3(sp)$	1.535248
52	$\Delta_{vaporization}H_m{}^{52}$	H attached to heteroatom	5.262695
53	$\Delta_{vaporization}H_m{}^{53}$	H^a attached to $C^0(sp^3)$ with 1X attached to next C	-0.00264
54	$\Delta_{vaporization}H_m{}^{54}$	H^a attached to $C^0(sp^3)$ with 4X attached to next C	-0.25246
55	$\Delta_{vaporization}H_m{}^{55}$	phenol or enol or carboxyl OH	5.864801
56	$\Delta_{vaporization}H_m{}^{56}$	=O	7.082408

57	$\Delta_{vaporization}H_m^{57}$	O--[b]		3.925496
58	$\Delta_{vaporization}H_m^{58}$	O- (negatively charged)		14.63773
59	$\Delta_{vaporization}H_m^{59}$	R-O-O-R		0.929495
60	$\Delta_{vaporization}H_m^{60}$	Al_2-NH		-10.547
61	$\Delta_{vaporization}H_m^{61}$	Ar-NH_2 or X-NH_2		-9.17802
62	$\Delta_{vaporization}H_m^{62}$	RCO-N< or >N-X=X		14.50506
63	$\Delta_{vaporization}H_m^{63}$	Ar_2NH or Ar_3N or Ar_2N-Al or R..N..R[c]		11.61996
64	$\Delta_{vaporization}H_m^{64}$	N+ (positively charged)		-6.55652
65	$\Delta_{vaporization}H_m^{65}$	F[a] attached to $C^1(sp^3)$		2.557539
66	$\Delta_{vaporization}H_m^{66}$	Cl[a] attached to $C^1(sp^3)$		2.299679
67	$\Delta_{vaporization}H_m^{67}$	R-SH		23.92881
68	$\Delta_{vaporization}H_m^{68}$	R2S / RS-SR		10.70825
69	$\Delta_{vaporization}H_m^{69}$	R=S		8.604026
70	$\Delta_{vaporization}H_m^{70}$	R_3-P=X		-4.94383
71	$\Delta_{vaporization}H_m^{71}$	PX_3 (phosphite)		11.11212
72	$\Delta_{vaporization}H_m^{72}$	presence (0) or absence (1) of C-C		-0.51537
73	$\Delta_{vaporization}H_m^{73}$	presence (0) or absence (1) of C-S		-2.68539
74	$\Delta_{vaporization}H_m^{74}$	presence (0) or absence (1) of N-N		-8.37556
75	$\Delta_{vaporization}H_m^{75}$	presence (0) or absence (1) of N-O		8.484444
76	$\Delta_{vaporization}H_m^{76}$	presence (0) or absence (1) of O-O		3.212364
77	$\Delta_{vaporization}H_m^{77}$	presence (0) or absence (1) of P-Cl		2.209483
78	$\Delta_{vaporization}H_m^{78}$	presence (0) or absence (1) of C-A-O	A means any atom	3.183966
79	$\Delta_{vaporization}H_m^{79}$	presence (0) or absence (1) of C-A-P	A means any atom	9.016153
80	$\Delta_{vaporization}H_m^{80}$	presence (0) or absence (1) of N-A-O	A means any atom	-3.20031
81	$\Delta_{vaporization}H_m^{81}$	presence (0) or absence (1) of N-A-Cl	A means any atom	4.836001
82	$\Delta_{vaporization}H_m^{82}$	presence (0) or absence (1) of O-A-O	A means any atom	-4.11953
83	$\Delta_{vaporization}H_m^{83}$	presence (0) or absence (1) of P-A-F	A means any atom	-15.3171
84	$\Delta_{vaporization}H_m^{84}$	presence (0) or absence (1) of Br-A-Br	A means any atom	-1.40065

85	$\Delta_{vaporization}H_m^{85}$	presence (0) or absence (1) of C-A1-A2-N	A1 and A2 means any atom	-0.79062
86	$\Delta_{vaporization}H_m^{86}$	presence (0) or absence (1) of C-A1-A2-O	A1 and A2 means any atom	1.164372
87	$\Delta_{vaporization}H_m^{87}$	presence (0) or absence (1) of F-A1-A2-Br	A1 and A2 means any atom	-5.46109
88	$\Delta_{vaporization}H_m^{88}$	presence (0) or absence (1) of Cl-A1-A2-Cl	A1 and A2 means any atom	-2.61117
89	$\Delta_{vaporization}H_m^{89}$	presence (0) or absence (1) of Br-A1-A2-Br	A1 and A2 means any atom	-3.27952
90	$\Delta_{vaporization}H_m^{90}$	presence (0) or absence (1) of C-A1-A2-A3-N	A1 , A2 and A3, means any atom	0.679808
91	$\Delta_{vaporization}H_m^{91}$	presence (0) or absence (1) of C-A1-A2-A3-O	A1 , A2 and A3, means any atom	-0.24364
92	$\Delta_{vaporization}H_m^{92}$	presence (0) or absence (1) of C-A1-A2-A3-F	A1 , A2 and A3, means any atom	1.680153
93	$\Delta_{vaporization}H_m^{93}$	presence (0) or absence (1) of S-A1-A2-A3-P	A1 , A2 and A3, means any atom	8.701483
94	$\Delta_{vaporization}H_m^{94}$	presence (0) or absence (1) of N-A1-A2-A3-A4-O	A1 , A2 and A3, means any atom	6.223277
95	$\Delta_{vaporization}H_m^{95}$	presence (0) or absence (1) of O-A1-A2-A3-A4-O	A1 , A2 , A3, and A4 means any atom	3.394989
96	$\Delta_{vaporization}H_m^{96}$	presence (0) or absence (1) of F-A1-A2-A3-A4-Cl	A1 , A2 , A3, and A4 means any atom	0.675476
97	$\Delta_{vaporization}H_m^{97}$	presence (0) or absence (1) of C-A1-A2-A3-A4-A5-N	A1 , A2 , A3, and A4 means any atom	-0.8111
98	$\Delta_{vaporization}H_m^{98}$	presence (0) or absence (1) of N-A1-A2-A3-A4-A5-F	A1 , A2 , A3, A4 and A5 means any atom	-4.89802
99	$\Delta_{vaporization}H_m^{99}$	presence (0) or absence (1) of F-A1-A2-A3-A4-A5-Cl	A1 , A2 , A3, A4 and A5 means any atom	-5.70174
100	$\Delta_{vaporization}H_m^{100}$	presence (0) or absence (1) of C-A1-A2-A3-A4-A5-A6-O	A1 , A2 , A3, A4 and A5 means any atom	-0.68942
101	$\Delta_{vaporization}H_m^{101}$	presence (0) or absence (1) of C-A1-A2-A3-A4-A5-A6-A7-Cl	A1 , A2 , A3, A4 ,A5 and A6 means any atom	-1.85662
102	$\Delta_{vaporization}H_m^{102}$	presence (0) or absence (1) of O-A1-A2-A3-A4-A5-A6-A7-A8-O	A1 , A2 , A3, A4 ,A5 ,A6 ,A7 and A8 means any atom	3.479901
103	$\Delta_{vaporization}H_m^{103}$	presence (0) or absence (1) of Cl-A1-A2-A3-A4-A5-A6-A7-A8-Cl	A1 , A2 , A3, A4 ,A5 ,A6 ,A7 and A8 means any atom	3.906784
104	$\Delta_{vaporization}H_m^{104}$	presence (0) or absence (1) of C-A1-A2-A3-A4-A5-A6-A7-A8-A9-O	A1 , A2 , A3, A4 ,A5 ,A6 ,A7 and A8 means any atom	4.874252
105	$\Delta_{vaporization}H_m^{105}$	presence (0) or absence (1) of C-A1-A2-A3-A4-A5-A6-A7-A8-A9-Cl	A1 , A2 , A3, A4 ,A5 ,A6 ,A7, A8 and A9 means any atom	5.893979
106	$\Delta_{vaporization}H_m^{106}$	number of C-C		4.340273
107	$\Delta_{vaporization}H_m^{107}$	number of C-N		5.088229
108	$\Delta_{vaporization}H_m^{108}$	number of C-O		2.860265
109	$\Delta_{vaporization}H_m^{109}$	number of C-S		3.068132
110	$\Delta_{vaporization}H_m^{110}$	number of C-P		10.07875

111	$\Delta_{vaporization}H_m^{111}$	number of C-Cl		6.329015
112	$\Delta_{vaporization}H_m^{112}$	number of C-Br		12.98586
113	$\Delta_{vaporization}H_m^{113}$	number of C-I		17.03061
114	$\Delta_{vaporization}H_m^{114}$	number of N-N		11.03813
115	$\Delta_{vaporization}H_m^{115}$	number of N-P		-7.74524
116	$\Delta_{vaporization}H_m^{116}$	number of C-A-O	A means any atom	-0.17862
117	$\Delta_{vaporization}H_m^{117}$	number of C-A-P	A means any atom	-1.27335
118	$\Delta_{vaporization}H_m^{118}$	number of C-A-Cl	A means any atom	0.6032
119	$\Delta_{vaporization}H_m^{119}$	number of N-A-S	A means any atom	6.758255
120	$\Delta_{vaporization}H_m^{120}$	number of N-A-F	A means any atom	0.855748
121	$\Delta_{vaporization}H_m^{121}$	number of O-A-O	A means any atom	3.258076
122	$\Delta_{vaporization}H_m^{122}$	number of C-A1-A2-C	A1 and A2 means any atom	0.251901
123	$\Delta_{vaporization}H_m^{123}$	number of C-A1-A2-O	A1 and A2 means any atom	-0.62205
124	$\Delta_{vaporization}H_m^{124}$	number of C-A1-A2-S	A1 and A2 means any atom	-0.23899
125	$\Delta_{vaporization}H_m^{125}$	number of C-A1-A2-Br	A1 and A2 means any atom	-1.04179
126	$\Delta_{vaporization}H_m^{126}$	number of C-A1-A2-I	A1 and A2 means any atom	-1.08473
127	$\Delta_{vaporization}H_m^{127}$	number of N-A1-A2-O	A1 and A2 means any atom	-0.85753
128	$\Delta_{vaporization}H_m^{128}$	number of O-A1-A2-O	A1 and A2 means any atom	0.312412
129	$\Delta_{vaporization}H_m^{129}$	number of O-A1-A2-Cl	A1 and A2 means any atom	-0.8331
130	$\Delta_{vaporization}H_m^{130}$	number of O-A1-A2-Br	A1 and A2 means any atom	-3.32737
131	$\Delta_{vaporization}H_m^{131}$	number of F-A1-A2-Cl	A1 and A2 means any atom	-0.56306
132	$\Delta_{vaporization}H_m^{132}$	number of C-A1-A2-A3-C	A1 , A2 and A3, means any atom	-0.30958
133	$\Delta_{vaporization}H_m^{133}$	number of C-A1-A2-A3-N	A1 , A2 and A3, means any atom	-0.9727
134	$\Delta_{vaporization}H_m^{134}$	number of C-A1-A2-A3-O	A1 , A2 and A3, means any atom	-0.61233
135	$\Delta_{vaporization}H_m^{135}$	number of C-A1-A2-A3-S	A1 , A2 and A3, means any atom	-0.536
136	$\Delta_{vaporization}H_m^{136}$	number of C-A1-A2-A3-F	A1 , A2 and A3, means any atom	-0.04273
137	$\Delta_{vaporization}H_m^{137}$	number of C-A1-A2-A3-Cl	A1 , A2 and A3, means any atom	-0.35663
138	$\Delta_{vaporization}H_m^{138}$	number of N-A1-A2-A3-A4-O	A1 , A2 , A3, and A4 means any atom	-0.39737

139	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{139}$	number of O-A1-A2-A3-A4-F	A1 , A2 , A3, and A4 means any atom	-2.46101
140	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{140}$	number of F-A1-A2-A3-A4-Cl	A1 , A2 , A3, and A4 means any atom	-0.94376
141	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{141}$	number of C-A1-A2-A3-A4-A5-C	A1 , A2 , A3, A4 and A5 means any atom	0.001966
142	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{142}$	number of C-A1-A2-A3-A4-A5-O	A1 , A2 , A3, A4 and A5 means any atom	-0.33009
143	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{143}$	number of C-A1-A2-A3-A4-A5-P	A1 , A2 , A3, A4 and A5 means any atom	-1.44459
144	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{144}$	number of Cl-A1-A2-A3-A4-A5-Cl	A1 , A2 , A3, A4 and A5 means any atom	-2.32488
145	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{145}$	number of C-A1-A2-A3-A4-A5-A6-A7-N	A1 , A2 , A3, A4 ,A5 ,A6 and A7 means any atom	-1.16851
146	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{146}$	number of Cl-A1-A2-A3-A4-A5-A6-A7-Cl	A1 , A2 , A3, A4 ,A5 ,A6 and A7 means any atom	2.143098
147	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{147}$	number of C-A1-A2-A3-A4-A5-A6-A7-A8-C	A1 , A2 , A3, A4 ,A5 ,A6 ,A7 and A8 means any atom	0.268851
148	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{148}$	number of C-A1-A2-A3-A4-A5-A6-A7-A8-F	A1 , A2 , A3, A4 ,A5 ,A6 ,A7 and A8 means any atom	0.461501
149	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{149}$	number of O-A1-A2-A3-A4-A5-A6-A7-A8-O	A1 , A2 , A3, A4 ,A5 ,A6 ,A7 and A8 means any atom	1.649915
150	$\Delta_{\mathrm{vaporization}}H_{\mathrm{m}}^{150}$	number of C-A1-A2-A3-A4-A5-A6-A7-A8-A9-O	A1 , A2 , A3, A4 ,A5 ,A6 ,A7, A8 and A9 means any atom	-3.05163

X represents any electronegative atom (O, N, S, P, Se, halogens);

Al and Ar represent aliphatic and aromatic groups, respectively;

= represents a double bond;

represents a triple bond;

-- represents an aromatic bond as in benzene or delocalized bonds such as the N-O bond in a nitro group

.. represents aromatic single bonds as the C-N bond in pyrrole

[a] The superscript represents the formal oxidation number. The formal oxidation number of a carbon atom equals the sum of the conventional bond orders with electronegative atoms; the C--N bond order in pyridine may be considered as 2 while we have one such bond and 1.5 when we have two such bonds; the C..X bond order in pyrrole or furan may be considered as 1.

[b] As in nitro, *N*-oxides

[c] Pyrrole-type structure.

Table 3-The elemental analysis of the model results

Chemical Family	%AARD	N
Hydrocarbons	2.4	689
Nitrogen compounds	4.7	504
Oxygenated compounds	4.5	1425
Phosphorous-containing compounds	2.7	41
Sulfur-containing compounds	3.6	163
Fluorine-containing compounds	4.4	204
Chlorine-containing compounds	3.7	211
Bromine-containing compounds	2.5	55
Iodine-containing compounds	1.8	34

Table 4- Comparison between the presented model and the models proposed by Ducros et al. [32, 33], Guthrie and Taylor [36], Chickos et al. [28], Domalski and Hearing [165] , Constantinou and Gani [29], and Kolská et al. [37], using the data set comprised of 83 compounds used in Santos and Leal [46] studies.

No.	Compound	exp.	This work			Santos and Leal		Ducrosa et al.		Guthrie and Taylor		Chickosc et al.		Domalskid et al.		Constantinoue and Gani		Kolskáf et al.	
			This work	AE	%ARD	AE	%AARD	AE	%ARD	AE	%ARD	AE	%ARD	AE	%ARD	AE	%ARD	AE	%ARD
1	3,3-Diethylpentane	42.6	43.5	0.9	2.1	1.1	2.6	0.1	0.2	0.7	1.6	2.9	6.8	0.4	0.9	0.6	1.4	0.2	0.5
2	2,2,4-Trimethylhexane	40.7	40.3	0.4	0.9	0.1	0.3	0.5	1.2	1.3	3.2	3.1	7.6	0.9	2.2	0.7	1.7	0.7	1.7
3	2,2,5-Trimethylhexane	40.2	40.7	0.5	1.2	0.1	0.3	1.0	2.5	1.8	4.5	2.6	6.5	1.4	3.5	0.1	0.3	0.3	0.8
4	2,3,5-Trimethylhexane	41.4	41.5	0.1	0.3	0.5	1.2	0.9	2.2	1.3	3.1	2.5	6.0	0.9	2.2	0.6	1.5	0.3	0.7
5	Nonane	46.4	46.1	0.3	0.7	0.3	0.7	0.3	0.7	0.4	0.9	1.3	2.8	0.0	0.0	1.2	2.6	0.9	1.9
6	2,4-Dimethyloctane	47.1	47.3	0.2	0.4	0.6	1.3	1.4	3.0	2.0	4.3	1.5	3.2	1.7	3.6	0.6	1.3	0.1	0.2
7	2-Methylnonane	49.6	49.2	0.4	0.8	0.3	0.6	0.2	0.4	0.9	1.8	1.9	3.8	0.5	1.0	0.5	1.0	0.1	0.2
8	Decane	51.4	51.1	0.3	0.6	0.4	0.8	0.3	0.6	0.5	1.0	1.6	3.1	0.1	0.2	0.9	1.8	0.6	1.2
9	Dodecane	61.5	61.1	0.4	0.7	0.9	1.5	0.4	0.7	0.5	0.8	2.3	3.7	0.2	0.3	0.1	0.2	0.1	0.2
10	Tri-tert-butylmethane	55.3	48.5	6.8	12.4	3.5	6.3	1.5	2.7	0.0	0.0	9.9	17.9	1.4	2.5	7.0	12.7	6.1	11.0
11	5-Ethyl-5-methyldecane	60.5	61.5	1.0	1.7	2.0	3.3	1.9	3.1	3.1	5.1	2.1	3.5	2.7	4.5	1.3	2.2	0.8	1.3
12	3,3,6,6-Tetraethyloctane	74.3	72.8	1.5	2.1	1.6	2.2	0.6	0.8	1.0	1.4	7.3	9.8	1.0	1.4	3.0	4.0	3.6	4.9
13	Hexadecane	81.4	81.0	0.4	0.4	1.4	1.7	0.4	0.5	0.9	1.1	3.5	4.3	0.7	0.9	1.2	1.5	1.1	1.4
14	2,4,4-Trimethyl-2-pentene	37.5	35.7	1.8	4.9	0.2	0.5	0.7	1.9	0.3	0.8	2.5	6.7	0.5	1.3	1.1	2.9	1.0	2.7
15	(Z)-2,2-Dimethyl-3-hexene	37.2	36.7	0.5	1.4	0.1	0.3	0.7	1.9	0.2	0.5	2.2	5.9	0.2	0.5	1.3	3.5	0.4	1.1
16	(E)-2,2-Dimethyl-3-hexene	37.2	36.7	0.5	1.4	0.3	0.8	0.7	1.9	0.2	0.5	2.2	5.9	0.4	1.1	1.3	3.5	0.4	1.1
17	1-Octene	40.4	40.3	0.1	0.2	0.0	0.0	0.1	0.3	0.5	1.2	0.1	0.3	0.0	0.0	0.1	0.3	0.6	1.5
18	(Z)-2-Octene	40.2	40.5	0.3	0.7	1.0	2.5	1.3	3.2	2.3	5.7	0.3	0.8	0.8	2.0	0.4	1.0	1.2	3.0
19	(E)-2-Octene	40.2	40.5	0.3	0.7	1.3	3.2	1.3	3.2	2.3	5.7	0.3	0.8	1.2	3.0	0.4	1.0	1.2	3.0

20	(Z)-3-Octene	39.7	40.5	0.8	1.9	1.2	3.0	1.9	4.8	3.3	8.3	0.8	2.0	1.0	2.5	0.6	1.5	1.5	3.8
21	(E)-3-Octene	40.2	40.5	0.3	0.7	1.0	2.5	1.4	3.5	2.8	7.0	0.3	0.8	0.9	2.2	0.1	0.3	1.0	2.5
22	(Z)-4-Octene	39.7	40.5	0.8	1.9	1.2	3.0	1.9	4.8	3.3	8.3	0.8	2.0	1.0	2.5	0.6	1.5	1.5	3.8
23	(E)-4-Octene	42.9	40.5	2.4	5.7	1.7	4.0	1.3	3.0	0.1	0.2	2.4	5.6	1.8	4.2	2.6	6.1	1.7	4.0
24	2,6-Dimethyl-1-heptene	45.9	43.1	2.8	6.1	2.3	5.0	1.3	2.8	1.0	2.2	2.8	6.1	1.9	4.1	3.4	7.4	3.0	6.5
25	1-Nonene	44.7	45.1	0.4	0.8	0.5	1.1	0.8	1.8	1.2	2.7	0.4	0.9	0.8	1.8	0.5	1.1	1.0	2.2
26	1-Decene	50.4	50.1	0.3	0.7	0.3	0.6	0.1	0.2	0.6	1.2	0.6	1.2	0.2	0.4	0.6	1.2	0.0	0.0
27	3-Methyl-3-propyl-1-heptene	50.9	50.8	0.1	0.2	1.0	2.0	0.9	1.8	0.4	0.8	1.9	3.7	1.7	3.3	0.1	0.2	0.2	0.4
28	1-Undecene	54.3	55.1	0.8	1.4	0.6	1.1	1.2	2.2	1.8	3.3	0.2	0.4	1.4	2.6	0.2	0.4	0.8	1.5
29	1-Dodecene	60.8	60.0	0.8	1.2	1.1	1.8	0.3	0.5	0.3	0.5	1.6	2.6	0.0	0.0	1.7	2.8	0.9	1.5
30	1-Hexadecene	80.2	80.0	0.2	0.2	1.1	1.4	0.2	0.3	1.2	1.5	2.3	2.9	1.0	1.3	2.5	3.1	1.4	1.8
31	1,5-Hexadiyne	31.9	35.4	3.5	11.1	1.4	4.4	3.5	11.0	31.9	100.0	0.8	2.5	6.9	21.6	0.3	0.9	0.7	2.2
32	(Z)-1,3,5-Hexatriene	34.1	31.7	2.4	7.1	1.1	3.2	0.5	1.5	25.7	75.4	3.0	8.8	1.0	2.9	2.4	7.0	3.8	11.1
33	1,7-Octadiyne	41.7	44.9	3.2	7.6	1.3	3.1	3.7	8.9	31.6	75.8	1.2	2.9	7.3	17.5	0.8	1.9	0.3	0.7
34	Bicyclopropyl	31.7	33.9	2.2	6.9	3.3	10.4	5.8	18.3	5.3	16.7	0.6	1.9	14.6	46.1	0.7	2.2	2.8	8.8
35	1-Cyclopropylpenta-1,3-diyne	51.9	50.0	1.9	3.7	1.2	2.3	41.0	79.0	41.8	80.5	11.4	22.0	32.3	62.2	5.9	11.4	5.7	11.0
36	1,1,2-Trimethylcyclopentane	38.1	36.6	1.5	4.0	0.5	1.3	0.4	1.1	2.5	6.6	3.1	8.1	6.1	16.0	0.5	1.3	2.5	6.6
37	1,1,3-Trimethylcyclopentane	36.6	35.4	1.2	3.1	0.1	0.3	1.1	3.0	1.0	2.7	0.5	1.4	4.6	12.6	0.0	0.0	2.9	7.9
38	Butylcyclopentane	45.9	45.6	0.3	0.7	0.3	0.7	0.4	0.9	1.7	3.7	0.8	1.7	5.3	11.6	0.3	0.7	0.2	0.4
39	1,1,3-Trimethylcyclohexane	41.9	39.5	2.4	5.7	0.6	1.4	0.1	0.2	1.2	2.9	0.1	0.2	0.9	2.2	0.9	2.2	4.2	10.0
40	1,1,4-Trimethylcyclohexane	45.6	40.1	5.5	12.0	4.3	9.4	3.8	8.3	4.9	10.8	3.8	8.3	2.8	6.1	1.0	2.2	7.9	17.3
41	Isopropylcyclohexane	44.0	44.2	0.2	0.4	0.2	0.5	0.1	0.2	1.2	2.7	0.9	2.1	0.9	2.1	0.3	0.7	0.3	0.7
42	Bicyclopentyl	50.4	49.4	1.0	2.0	1.4	2.8	1.0	2.0	3.8	7.5	0.6	1.2	10.5	20.8	2.0	4.0	0.1	0.2
43	tert-Butylcyclohexane	47.0	46.7	0.3	0.7	0.6	1.3	0.3	0.6	1.2	2.6	2.6	5.5	0.5	1.1	2.3	4.9	0.0	0.0
44	Bicyclohexyl	58.0	58.8	0.8	1.4	1.4	2.4	1.6	2.8	1.3	2.2	1.2	2.1	3.5	6.0	0.9	1.6	0.5	0.9
45	Decylcyclohexane	78.7	80.5	1.8	2.3	0.3	0.4	1.5	1.9	0.9	1.1	0.8	1.0	3.3	4.2	0.9	1.1	0.6	0.8
46	Dodecylcyclohexane	88.9	90.5	1.6	1.8	0.3	0.3	1.3	1.5	0.8	0.9	1.6	1.8	3.3	3.7	1.8	2.0	1.4	1.6
47	3-Isopropyl-6-methylene cyclohexene	49.2	50.3	1.1	2.2	1.0	2.0	2.6	5.3	10.0	20.3	1.5	3.1	4.2	8.5	3.8	7.7	1.1	2.2
48	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	53.2	52.0	1.2	2.3	1.0	1.9	3.2	6.0	5.2	9.8	3.4	6.4	1.6	3.0	5.3	10.0	4.0	7.5
49	1,3-Dimethylcyclopentene	35.0	36.5	1.5	4.4	0.4	1.1	1.8	5.1	1.8	5.1	0.8	2.3	3.6	10.3	0.4	1.1	4.7	13.4

50	1,4-Dimethylcyclopentene	34.5	36.5	2.0	5.9	0.1	0.3	2.8	8.1	1.1	3.2	1.3	3.8	4.1	11.9	0.6	1.7	5.2	15.1
51	1,5-Dimethylcyclopentene	36.5	37.1	0.6	1.6	1.4	3.8	0.3	0.8	0.3	0.8	2.8	7.7	2.1	5.8	1.0	2.7	4.3	11.8
52	4-Ethylcyclopentene	36.8	36.6	0.2	0.5	0.1	0.3	0.1	0.3	1.5	4.1	1.0	2.7	2.0	5.4	3.2	8.7	1.1	3.0
53	3-Methylcyclohexene	38.8	36.6	2.2	5.6	3.1	8.0	2.0	5.2	2.3	5.9	3.0	7.7	1.0	2.6	4.7	12.1	1.4	3.6
54	1-Methyl-4-isopropyl-1,4-cyclohexadiene	51.4	51.3	0.1	0.1	0.6	1.2	8.7	16.9	9.6	18.7	3.7	7.2	2.3	4.5	5.7	11.1	1.1	2.1
55	1-Ethenyl-2-methylbenzene	49.3	48.0	1.3	2.7	0.0	0.0	10.7	21.7	12.4	25.2	6.2	12.6	3.1	6.3	3.3	6.7	0.1	0.2
56	1-Ethenyl-3-methylbenzene	49.5	47.7	1.8	3.6	0.8	1.6	11.8	23.8	12.6	25.5	4.4	8.9	2.0	4.0	3.1	6.3	0.5	1.0
57	1-Ethenyl-4-methylbenzene	48.9	48.0	0.9	1.8	0.2	0.4	11.7	23.9	12.0	24.5	3.8	7.8	0.7	1.4	3.7	7.6	1.7	3.5
58	(Z)-1-Propenylbenzene	49.1	47.4	1.7	3.4	0.4	0.8	10.1	20.6	10.2	20.8	4.0	8.2	0.5	1.0	2.5	5.1	2.4	4.9
59	(E)-1-Propenylbenzene	46.9	47.4	0.5	1.1	2.9	6.2	7.9	16.8	8.0	17.1	1.8	3.8	3.1	6.6	4.7	10.0	4.6	9.8
60	Allylbenzene	46.2	46.4	0.2	0.5	0.0	0.0	3.9	8.4	4.2	9.1	1.1	2.4	3.6	7.8	2.4	5.2	0.2	0.4
61	1-Ethyl-2-ethenylbenzene	52.1	52.3	0.2	0.5	2.0	3.8	9.3	17.9	11.8	22.7	4.4	8.5	2.5	4.8	5.0	9.6	1.1	2.1
62	1-Ethyl-3-ethenylbenzene	53.9	52.4	1.5	2.8	0.4	0.7	12.1	22.5	13.6	25.2	4.1	7.6	2.9	5.4	3.2	5.9	0.1	0.2
63	1-Ethyl-4-ethenylbenzene	52.6	52.7	0.1	0.2	0.9	1.7	11.3	21.5	12.3	23.4	2.8	5.3	1.0	1.9	4.5	8.6	1.9	3.6
64	1-Buten-2-ylbenzene	51.8	51.8	0.0	0.1	2.1	4.1	8.0	15.5	8.3	16.0	2.0	3.9	4.4	8.5	3.6	7.0	2.9	5.6
65	(3-Methyl-1-buten-2-yl) benzene	53.2	54.9	1.7	3.2	3.4	6.4	6.3	11.8	4.8	9.0	0.8	1.5	2.0	3.8	5.5	10.3	4.2	7.9
66	3-Methyl-1-tert-butylbenzene	51.1	53.4	2.3	4.5	1.5	2.9	2.8	5.5	1.0	2.0	2.1	4.1	0.3	0.6	7.4	14.5	0.3	0.6
67	4-Methyl-1-tert-butylbenzene	52.2	53.7	1.5	2.9	0.4	0.8	1.2	2.3	0.1	0.2	3.2	6.1	0.2	0.4	6.3	12.1	0.3	0.6
68	(3,3-Dimethyl-1-buten- 2-yl) benzene	53.2	57.4	4.2	7.9	7.0	13.2	3.2	6.0	5.1	9.6	0.5	0.9	0.9	1.7	7.1	13.3	6.6	12.4
69	Cyclohexylbenzene	60.8	60.7	0.1	0.2	1.6	2.6	0.7	1.2	1.8	3.0	1.6	2.6	0.4	0.7	2.3	3.8	1.6	2.6
70	3,5-Dimethyl-1-tert-butylbenzene	56.6	57.9	1.3	2.4	0.8	1.4	2.4	4.2	0.2	0.4	2.9	5.1	2.3	4.1	7.5	13.2	1.1	1.9
71	1,3,5-Triethylbenzene	59.2	61.7	2.5	4.3	2.3	3.9	1.0	1.7	1.5	2.5	0.0	0.0	4.2	7.1	2.8	4.7	0.3	0.5
72	1,3-Di-isopropylbenzene	56.2	58.7	2.5	4.5	0.7	1.3	0.6	1.1	0.3	0.5	1.2	2.1	1.6	2.9	1.7	3.0	0.9	1.6
73	1,4-Di-isopropylbenzene	56.5	59.0	2.5	4.4	1.0	1.8	0.2	0.4	0.0	0.0	1.5	2.7	1.3	2.3	1.4	2.5	0.7	1.2
74	1,3-Di-tert-butylbenzene	59.6	63.6	4.0	6.8	3.3	5.5	5.6	9.4	1.5	2.5	2.0	3.4	1.6	2.7	14.5	24.3	0.1	0.2
75	1,4-Di-tert-butylbenzene	63.0	63.9	0.9	1.5	0.1	0.2	1.7	2.7	1.9	3.0	5.4	8.6	1.2	1.9	11.1	17.6	2.7	4.3
76	1,3,5-Tri-isopropylbenzene	64.6	71.0	6.4	9.9	2.3	3.6	4.4	6.8	3.3	5.1	2.4	3.7	0.6	0.9	6.6	10.2	0.9	1.4
77	1,2,4,5-Tetra-isopropylbenzene	75.7	82.3	6.6	8.7	3.9	5.2	7.0	9.3	3.6	4.8	0.9	1.2	4.4	5.8	8.8	11.6	2.1	2.8
78	1,1-Diphenylethylene	71.2	71.4	0.2	0.3	2.9	4.1	9.9	13.9	11.0	15.5	2.6	3.7	2.0	2.8	9.2	12.9	7.1	10.0
79	(Z)-1,2-Diphenylethylene	70.5	72.7	2.2	3.1	3.9	5.5	14.0	19.9	14.4	20.4	1.9	2.7	7.9	11.2	10.5	14.9	9.6	13.6

80	(E)-1,2-Diphenylethylene	79.6	72.7	6.9	8.7	2.5	3.1	23.1	29.0	23.5	29.5	11.0	13.8	0.8	1.0	1.4	1.8	0.5	0.6
81	1,1-Diphenylethane	68.9	70.3	1.4	2.1	3.8	5.5	1.4	2.0	2.1	3.1	2.4	3.5	23.3	33.8	4.4	6.4	4.3	6.2
82	2-Methyl-1,1-diphenylpropane	73.2	76.9	3.7	5.0	0.7	1.0	5.8	7.9	6.6	9.0	2.7	3.7	27.9	38.1	7.3	10.0	7.0	9.6
83	Tri-phenylethene	91.8	100.5	8.7	9.5	13.0	14.2	7.1	7.7	7.7	8.4	4.9	5.3	15.8	17.2	23.4	25.5	20.1	21.9
	Total			1.6	3.1	1.4	2.6	3.7	7.0	5.1	10.6	2.4	4.6	3.3	6.4	3.1	5.5	2.1	4.1

Research Highlights

- A new group contribution model is presented for the estimation of vaporization enthalpy.
- A compendium of experimental data for 2811 compounds is used to develop and validate the model.
- The model shows low deviation from experimental data.