Journal of chemical & engineering data

Article

Cite This: J. Chem. Eng. Data 2018, 63, 4735−4740

pubs.acs.org/jced

An Improved Quantitative Structure Property Relationship Model for Predicting Thermal Conductivity of Liquid Aliphatic Alcohols

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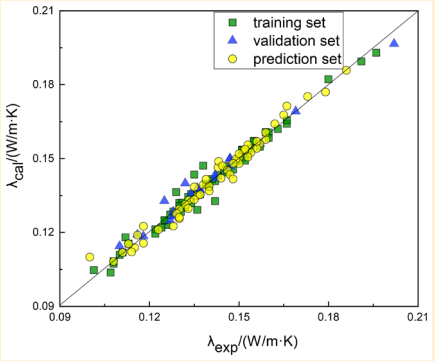
Supporting Information

ABSTRACT: The quantitative structure property relationship (QSPR) for thermal conductivity of liquid aliphatic alcohols was developed on the basis of 139 thermal conductivity data points of liquid aliphatic alcohols, which were divided into a 65-member training set, a 20-member validation set, and a 54-member prediction set. Four parameters (temperature-*T*, the intrinsic state pseudoconnectivity index-type 1s-*Psi_i_1s*, the sixth eigenvalue from augmented edge adjacency matrix weighed by edge degree-*Eig06_AEA(ed)*, and the global topological charge index-*JGT*) were screened to develop the model by using the stepwise regression and the best subset regression method. For the training set, validation set and prediction set, the square correlation coefficient (R^2) is 0.9769, 0.9726, and 0.9738, respectively. The mean relative deviation values of training set, validation set, and prediction set were 1.4%, 1.6%, and 1.6%. The QSPR model can provide not only basic data for the engineering application but also theoretical guidance for designing and seeking specific thermal conductivity materials.



1. INTRODUCTION

Thermal conductivity is the essential physical property of chemicals and a fundamental property for the chemical industry, technological design, and energy engineering, and closely related to its composition, structure, density, pressure, and temperature.[1,2]

In the production process, people have developed many measuring methods in order to obtain thermal conductivity data. However, each measurement method has its limitation of applications. There are two reasons for this. One is that thermal convection and diffusion within fluids and the heat loss in experiments (especially at high temperatures) have not been solved, which make the measurement errors of liquid thermal conductivity very big. The other reason is that some compounds are easily decomposed and volatile, which makes thermal conductivity inaccessible in experiments. Therefore, the thermal conductivity data of many compounds is lacking.[3,4]

Under this circumstance, some calculation methods are deduced to predict thermal conductivity. The results of these methods for calculating thermal conductivity of alcohols are listed in Table 1. However, these methods are empirical, and they need experimental data to support. First and foremost, each formula's error in calculation is also relatively big, generally between 3 and 10%.

Table 1. Results of Some Empirical Methods for Calculating Thermal Conductivity of Alcohols

author	Rodenbush	Nagvekar	Baroncini et al.
no. of data point	267	634	592
MRD (%)	2.7	6.3	7.7
ref	5	6	7

Considering the limitation of empirical methods, some researchers have attempted to predict thermal conductivity of compounds based on QSPR models. They estimated the physical properties of compounds with molecular descriptors.[8−10] The possibility of estimation can be substantial and the accuracy in calculation can be increased.[11] The research on QSPR models for predicting thermal conductivity is listed in Table 2. It can be seen that using QSPR to predict the properties of organic compounds is simple and efficient.

At present, diverse linear and nonlinear methods are used to develop QSPR models.[16−20] Linear QSPR model can be used to reveal the parameters affecting the properties of compounds, and predict the properties of compounds simply and conveniently.

Aliphatic alcohol is an important category of organic compounds and an important raw material in daily life and chemical production, and thermal conductivity is an important data in the industrial production and utilization of such compounds.

The present work intends to (1) collect thermal conductivity data of liquid aliphatic alcohol from literatures and experiments; (2) extract and find out molecule characteristic

Received: August 28, 2018
Accepted: November 13, 2018
Published: November 29, 2018

DOI: 10.1021/acs.jced.8b00764
J. Chem. Eng. Data 2018, 63, 4735−4740

Table 2. Review of Previous Models for Predicting Properties about Thermal Conductivity

method	authors	compound class	parameters	n	R^2	result	ref
MLR[a]	Liu et al.	diverse organic compound	4	86	0.9620	RMSEP = 0.003	12
MLR	Cao et al.	alkanes	4	155	0.9510	s[c] = 0.0033	13
MLR	Kauffman et al.	organic solvents	9	213	0.8172	s = 0.0143	14
GFA[b]	Aboozar et al.	alcohols	5	155	0.9438	RMSE[d] = 0.0474	15

[a]Note: MLR stands for Multiple Linear Regression. [b]GFA stands for Genetic Function Approximation. [c]s stands for standard deviation; [d]RMSE stands for root-mean-square error.

descriptors that influence thermal conductivity; (3) develop a more robust and simpler linear QSPR model that could predict the thermal conductivity of liquid aliphatic alcohols effectively.

2. MATERIAL AND METHODS

2.1. Data Set Preparation. Thermal conductivity data of liquid aliphatic alcohols were collected from *Handbook of Thermal Conductivity of Liquids and Gases*.[4] A total of 114 experimental data collected covered a wide range of compounds (C1−C18) and temperature (280 K−450 K), which were divided into a 65-member training set, a 20-member validation set, and a 29-member prediction set, with stratified randomization method. Stratified randomization refers to the situation in which strata are constructed based on values of predicting variables, and a randomization scheme is performed separately in each stratum, therefore a balanced representation of a column's levels in each of the training, validation, and prediction sets is obtained.

To ensure the diversity of aliphatic alcohol present in the training set, validation set, and prediction set, the diversity test was performed using the Euclidean distance.[21] As shown in Figure 1, the scatter distribution indicates the diversity of the training set, validation set, and prediction set.

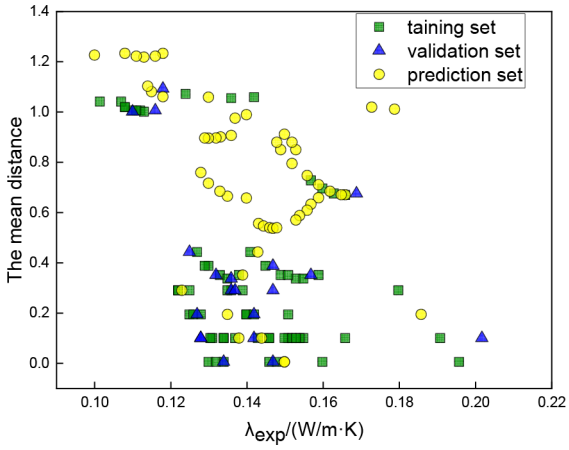


Figure 1. Similarity test of thermal conductivity.

To obtain more data to validate the predictive ability of the model, another 25 data were measured using the DRE-2A thermal conductivity instrument with nonequilibrium state hot-wire method. At first, the liquid sample (100 mL) was poured into the test tube, then, the probe was inserted into the test tube, and put it into the constant temperature water tank. After the probe and the sample achieved the heat balance, a certain amount of electric current was plugged into the probe, and the temperature of it rose, and then the heat was transferred to the liquid, and in turn the temperature decreased. According to the relationship between temperature and time, thermal conductivity was calculated automatically by the instrument. Each sample was measured three times and the final result is an averaged value. The error of measurement is < ±3%, and these measured data were included into the prediction set.

Finally, the database consisted of a 65-member training set, a 20-member validation set, and a 54-member prediction set, which were listed in Supporting Information (Table S1). The training set was used for model development, the validation set was used as the criteria for the model development, and the prediction set was used to evaluate the predictive ability of the developed model.

2.2. Molecular Descriptors Calculation and Screening. First, structures of aliphatic alcohols were constructed in the GaussView graphical interface software package.[22] And then, the structures were optimized using keywords (B3LYP/6-31G(d) opt freq) in Gaussian 09.[23] Finally the optimized molecular structures were input into Dragon6.0[24] software. The logical molecular descriptor blocks of topological indices, walk, and path counts, connectivity indices, 2D autocorrelation, edge adjacency indices, burden eigenvalues, P_VSA-like descriptors, and Randic molecular profiles, etc. for each molecule were calculated by Dragon.

Next, because constant and near-constant descriptors have no or little information, the presence of missing values can lead to missing molecular structure information, and the pair correlation among descriptors greater than 0.90 will lead to the multicollinearities of the model, the following descriptors were excluded: (i) descriptors with constant and near-constant values whose standard deviation are less than 0.001; (ii) descriptors with at least one missing value; (iii) descriptors with pair correlation larger than or equal to 0.90. As a result, 297 descriptors were retained.

2.3. QSPR Model Development. The stepwise regression method in DPS software package[25] was used to screen descriptors and establish the QSPR model. Using stepwise regression method, 9 descriptors were screened out. Best subset regression (BSR) can compare different regression models that contain subsets of the predictors, and it is an efficient way to identify models that adequately fit data with as few predictors as possible. Finally, a linear 4-descriptor QSPR model was developed by using BSR method with ordinary least-squares algorithm, including *T*, *Psi_i_1s*, *Eig06_AEA(Ed)*, and *JGT*. To avoid overfitting, the maximization correlation coefficient (Q^2) of the validation set acted as a criteria for the model developing, and the prediction set was used to estimate the predictive ability of the QSPR model. All data including descriptors and thermal conductivity are available in the Supporting Information (Table S1).

3. RESULTS AND DISCUSSION

The proposed QSPR model for the prediction of thermal conductivity of liquid aliphatic alcohols was developed:

DOI: 10.1021/acs.jced.8b00764
J. Chem. Eng. Data 2018, 63, 4735−4740

$$\lambda = 0.21460 + 0.10070Psi\_i\_1s - 0.06572JGT + 0.00988Eig06\_AEA(ed) - 0.00018T$$
$$(n_{training} = 65, \quad R^2_{training} = 0.9769,$$
$$RMSE_{training} = 0.0029, \quad n_{validation} = 20,$$
$$Q^2_{validation} = 0.9769, \quad RMSE_{validation} = 0.0033,$$
$$n_{prediction} = 54, \quad R^2_{prediction} = 0.9738,$$
$$RMSE_{prediction} = 0.0029, \quad Q^2_{F3} = 0.9767)$$

The model shows that the thermal conductivity is positively correlated with *JGT* and *Eig06_AEA(Ed)*, and negatively correlated with *Psi_i_1s* and *T*.

3.1. Model Validation. Model validation can evaluate the robustness and the predictive ability of the QSPR model.

Roberto Todeschini et al. (in 2016)[26] dealt with the evaluation of five Q^2 metrics (i.e., Q^2_{F1}, Q^2_{F2}, Q^2_{F3}, Q^2_{ccc}, and Q^2_{Rm}) and highlighted that only the Q^2_{F3} metric satisfies all the four fundamental mathematical principles. So, they strongly recommended using Q^2_{F3} as predictive ability metric. Q^2_{F3} was defined as the following:

$$Q^2_{F3} = 1 - \frac{\sum_{i=1}^{n_{OUT}} (y_i - \hat{y}_{i/i})^2 / n_{OUT}}{\sum_{i=1}^{n_{TR}} (y_i - \bar{y}_{TR})^2 / n_{TR}}$$

where y_i is the experimental response of the ith object, $\hat{y}_{i/i}$ is the predicted response when the ith object is not in the training set, n_{TR} and n_{OUT} are the number of training and prediction objects, respectively, and $\bar{y}_{TR}$ is the average value of the training set experimental responses. In their latest article, Roberto Todeschini et al. still suggested using RMSEP as a predictive metric based on the different training data set (in 2018).[27]

The value of Q^2_{F3} is 0.9767. RMSEP and other model statistics of QSPR model are listed in Table 3. From Table 3, it is apparent that $R^2 > 0.97$, $Q^2_{F3} > 0.98$, and RMSEP = 0.0029, which indicates that the QSPR model is acceptable.

Table 3. Model Statistics of All the Three Sets

data sets	n	$R^2(Q^2)$	s	RMSE(C/P)	MRD	F
training set	65	0.9769	0.0186	0.0029	1.4%	633.35
validation set	20	0.9726	0.0184	0.0033	1.6%	
prediction set	54	0.9738	0.0188	0.0029	1.6%	

Validation for each parameter is an essential step of QSPR modeling. According to the standardized coefficient, each parameter, and statistics are listed in Table 4.

The variance inflation factors (VIF) computed as VIF = $(1 - R^2) - 1$ (where R^2 is the coefficient of determination) can be used to identify whether high multicollinearities exist among the descriptors. As shown in Table 4, all the VIF values in the model were less than 2, which indicated that no multicollinearities exist.

Standardized coefficient can identify which of the independent variables have a greater effect on the dependent variable in a multiple regression analysis. From the standardized coefficient in Table 4, the most significant influence of the parameters on thermal conductivity in turn is *Psi_i_1s*, *JGT*, *Eig06_AEA(Ed)*, and *T*. The descriptors and their meaning are given in Table 5.

Table 5. Three Molecular Descriptors Used in QSPR Model

molecular descriptor	ref	type	definition
Psi_i_1s	28,29	topological indices	intrinsic state pseudoconnectivity index-type 1s
JGT	29,30	2D autocorrelations	global topological charge index
Eig06_AEA(Ed)	29	edge adjacency indices	sixth eigenvalue from augmented edge adjacency mat. weighted by edge degree
T			temperature

To make clear the relationship among molecules, descriptors, and thermal conductivity, Table 6 shows some examples of molecules, descriptors, and thermal conductivity values at 340 K. The other molecules, descriptors, and thermal conductivity values were listed in Table S1.

3.1.1. Psi_i_1s. Intrinsic state pseudoconnectivity index (*Psi_i_1s*)[29] is the most significant structural factor affecting the thermal conductivity of aliphatic alcohols, belonging to the topological index. It is defined as

$$I_i = \frac{(2/L_i)^2 \cdot \delta_i^v + 1}{\delta_i}$$
$$1\Psi_{1s} = \prod_b (I_i + I_j)_b^{-1/2}$$

where L_i is the main quantum number, δ_i^v is the valence electron number, i is the sigma electron number of the i atom, I_i is the intrinsic state of the ith atom, I_j is the intrinsic state of the jth atom, and b is the bond between the i atom and the j atom.

Psi_i_1s describes the intrinsic state of the molecule, the distribution of valence electrons and the energy density of the molecule. For alcohols with different numbers of carbon atoms, the larger the *Psi_i_1s* value is, the greater the energy density of the molecule is, and the higher the thermal conductivity is. For example, the *Psi_i_1s* values of methyl-1-hexanol and nonanol are 0.002 and 0.004. And their thermal conductivity values are 0.133 and 0.151.

3.1.2. JGT. The second parameter affecting the thermal conductivity of aliphatic alcohols is the global topological

Table 4. Statistical Validation Values for Each Parameter in the Regression Equation

parameter	coefficient	standardized coefficient	t-validation	P	VIF
Psi_i_1s	0.10070	0.005569	18.09	<0.0001	1.01
JGT	−0.06572	0.002057	−31.94	<0.0001	1.50
Eig06_AEA(Ed)	0.00988	0.000841	11.73	<0.0001	1.44
T	−0.00018	0.000013	−13.48	<0.0001	1.26

DOI: 10.1021/acs.jced.8b00764
J. Chem. Eng. Data 2018, 63, 4735−4740

Table 6. Some Examples of Aliphatic Alcohols at 340 K

name	structure	no. of carbon	*Psi_i_1s*	*JGT*	*Eig06_AEA(Ed)*	λ(W/m·K)
n-butyl alcohol	$CH_3(CH_2)_3OH$	4	0.065	0.262	0.000	0.143
tertiary butanol	$(CH_3)_3COH$	4	0.063	0.750	0.000	0.110
methyl-1-hexanol	$(CH_3)_2(CH_2)_4OH$	6	0.002	0.405	0.715	0.133
nonanol	$CH_3(CH_2)_8OH$	9	0.004	0.159	1.000	0.151

charge index *JGT*.[29,30] *JGT* belongs to a 2D-autocorrelation index calculated on the basis of the adjacency matrix of the molecular topology graph and the reciprocal squared distance matrix to describe the charge transfer between two atoms. Global topological charge index J is defined as

$$J = \sum_{k=1}^{5} J_k$$

where k is the path length and J_k is the average topology charge index, which is defined as

$$M = AD^{-2}$$

$$|CT_{ij}| = CT_{ij} = \begin{cases} \delta_i & \text{if } i = j \\ m_{ij} - m_{ji} & \text{if } i \neq j \end{cases}$$

$$G_k = \frac{1}{2} \cdot \sum_{i=1}^{A} \sum_{j=i+1}^{A} |CT_{ij}| \cdot \delta(d_{ij}; k)$$

$$J_k = \frac{G_k}{N}$$

where A is the adjacency matrix of the molecular topology graph, D^{-2} is the reciprocal squared distance matrix, m_{ij} is the element of matrix M, δ_i is the vertex degree of the i atom, N is the number of edges, and d_{ij} is the topological distance between the i atom and the j atom. If $d_{ij} \neq k$, $\delta(d_{ij}; k) = 1$. If $d_{ij} = k$, $\delta(d_{ij}; k) = 0$.

JGT describes the degree of molecular branches. The larger the *JGT* value is, the more molecular branches are, and the shorter the main chain is. Accordingly, heat transferring along the main chain is reduced, and so is thermal conductivity. The more molecular branches there are, the greater is the value of *JGT*, such as *JGT* values of *n*-butyl alcohol and tertiary butanol are 0.262 and 0.750, and their thermal conductivity values are 0.143 and 0.110.

3.1.3. Eig06_AEA(ed). The third parameter that affects the thermal conductivity of aliphatic alcohols is sixth eigenvalue from augmented edge adjacency matrix, weighted by edge degree (*Eig06_AEA(ed)*),[29] which is a topological index calculated on the basis of the edge adjacency matrix of the molecule. Weighted edge adjacency matrices ($EA(w)$) are unsymmetrical edge matrices derived from an edge weighted molecular graph obtained by applying an edge weighting scheme w, where *ed* represents the edge degree. By replacing the zero-diagonal elements of the edge adjacency matrix with specific key attributes, an edge-advanced adjacency matrix ($AEA(w)$) is obtained, each encoding a specific chemical information.

A weighted edge adjacency matrix wE can be calculated as

$$[wE]ij = \begin{cases} w_j & \text{if } (i, j) \text{ are adjacent bonds} \\ 0 & \text{otherwise} \end{cases}$$

The augmented edge adjacency matrix $aE(w)$ can be derived from an edge-weighted molecular graph, for any weighting scheme w as

$$[aE(w)]ij = \begin{cases} 1 & \text{if } (i, j) \text{ are adjacent bonds} \\ w_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

The *Eig06_AEA(Ed)* describes the expansion and contraction of the matrix. The larger are the eigenvalues, the greater is the scalability of the molecule, and the greater is the molecular vibration. Since molecular vibration contributes to heat conduction, the greater is the thermal conductivity.[31] For example, the *Eig06_AEA (ed)* values of methyl-1-hexanol and nonanol were 0.715 and 1, respectively. And their thermal conductivity values are 0.133 and 0.151.

The above three parameters describe the structural characteristics of the molecule from the degree of branching of aliphatic alcohols, energy density, and molecular scalability, and the combination has good correlation with thermal conductivity of liquid aliphatic alcohols. Besides these three parameters, temperature also has an effect on thermal conductivity.

3.1.4. Temperature (T). According to the experiments, the effect of temperature on the thermal conductivity of liquid compounds is remarkable. As the temperature rises, the movement of the molecules inside the liquid is more chaotic, and the molecular directional motion from the high energy area to the low energy area weakens, and heat conduction is reduced. Therefore, as the temperature increases, the thermal conductivity decreases.

These four parameters have a significant contribution to the thermal conductivity of aliphatic alcohols. The correlation between the calculated results and the experimental values is shown in Figure 2 and the calculated values were listed in Table S1.

Figure 2 shows that the calculated thermal conductivity values of the QSPR model were in high agreement with the experimental values.

3.2. Applicability Domain (AD). The Applicability Domain (AD) of a QSAR model is the information space on which the training set of the model has been developed. The purpose of AD is to testify whether the model can be reliably applicable. In general, this is the case for interpolation rather than for extrapolation.[21,32]

To visualize the AD of a QSPR model, the Williams plot of standardized crossvalidated residuals (R) versus leverage (Hat diagonal) values (h) can be used for a simple graphical detection of both the response outliers (i.e., compounds with crossvalidated standardized residuals greater than three standard deviation units, $R > 3\sigma$) and structurally influential chemicals in a model ($h > h^*$, $h^* = 3p/n$, where p is the number of model parameters plus one, and n is the number of the objects used to develop the model).

Figure 3 shows the Williams plot (AD) of the QSPR model.

DOI: 10.1021/acs.jced.8b00764
J. Chem. Eng. Data 2018, 63, 4735−4740

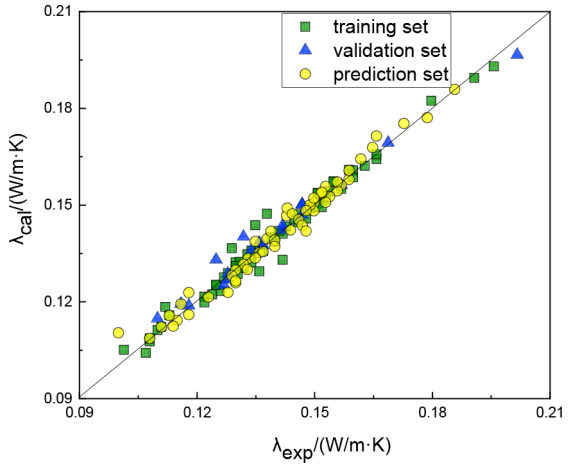


Figure 2. Calculated liquid thermal conductivity vs experimental values.

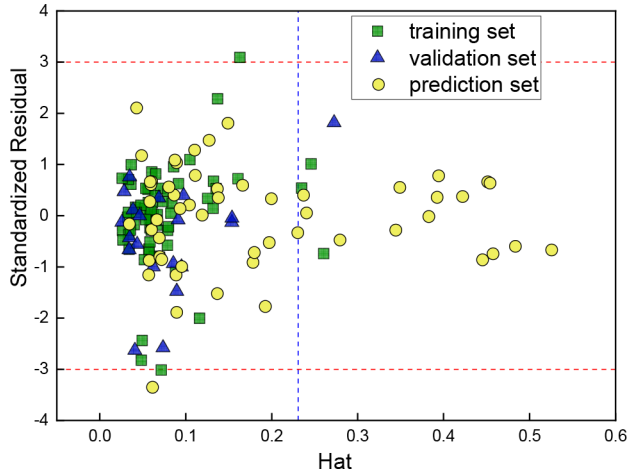


Figure 3. Applicability Domain of the proposed model.

The AD is mostly located in the region of $0 \leq h \leq 0.231$ (blue vertical line) and $-3 \leq R \leq 3$. Existence of the majority of data of training set, validation set, and prediction set points in this domain reveals that both model derivation and prediction are done in the applicability domain which results in a valid model. Good high leverage points are located in the domain of $h > 0.231$ and $-3 \leq R \leq 3$. These points fit the model well and make it more stable and precise.

The MRD values of training set, validation set, and prediction set were 1.4%, 1.6%, and 1.6%. Compared with those of earlier works, Rodenbush[5] (MRD is 2.7%), Negvekar[6] (MRD is 6.3%), Baroncini[7] (MRD is 7.7%), Liu et al.[12] (RMSEP = 0.003), Cao et al.[13] (R^2 is 0.9510), Kauffman et al.[14] (R^2 is 0.8172), and Aboozar et al.[15] (RMSE = 0.0474, R^2 = 0.9438), the present model exhibits superior performance.

In summary, the established QSPR model is not only robust but also has reliable predictive ability.

4. CONCLUSIONS

A four-parameter linear QSPR model was developed by using the stepwise regression method and the BSR method. The MRD values of training set, validation set, and prediction set were 1.4%, 1.6%, and 1.6%, respectively, within the range of experimental error (typically 5%). Besides high accuracy and significant correlation between molecular structure and the liquid thermal conductivity, the selected descriptors have explicit physical meanings and show that the liquid thermal conductivity depends on the degree of branching of liquid aliphatic alcohols, energy density, and molecular scalability. And most data points are located in the acceptable applicability domain, which means that the QSPR model is reliable and has high predictive ability. In addition, analyzing the model with various validation techniques verifies the reliability and robustness of the present model ($R^2 > 0.97$ and $Q^2_{F3} > 0.98$).

The study provides a convenient calculation method for calculating liquid thermal conductivity data of liquid aliphatic alcohols. It can provide fundamental data for the engineering application, as well as theoretical guidance for designing and seeking specific thermal conductivity materials.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jced.8b00764.

Values of molecular descriptors and thermal conductivity (PDF)

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Funding

The work was supported by the National Natural Science Foundation of China (No.2147204, 21672058, 21402048), and the Scientific Research Fund of Hunan Provincial Education Department (No.16B087).

Notes

The authors declare no competing financial interest.

■ NOMENCLATURE

Roman Symbols

R the correlation coefficient

T temperature

Greek Symbols

λ thermal conductivity

Sub- and Superscripts

calc calculated property

exp experimental property

Abbreviations

QSPR	quantitive structure property relationship
Psi_i_1s	intrinsic state pseudoconnectivity index
Eig06_AEA(ed)	sixth eigenvalue from augmented edge adjacency mat. weighted by edge degree
JGT	the global topological charge index
MRD	mean relative deviation
s	standard deviation
MLR	multiple linear regression
GFA	genetic function approximation
BSR	best subset regression
VIF	variance inflation factors

DOI: 10.1021/acs.jced.8b00764
J. Chem. Eng. Data 2018, 63, 4735−4740

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DOI: 10.1021/acs.jced.8b00764
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