# Molecular Volume and Density Models for Alkanes and Monoderivatives of Hydrocarbon

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## Abstract

**Motivation.** Eigenvalue of bonding orbital-connecting matrix is a good descriptor for expressing the relative bond energies of C-C and C-H bonds in alkanes. Its application can be extended to the Monoderivatives of Hydrocarbon.

**Method.** Multivariable models were developed to predict the densities of alkanes and monosubstituted alkanes. These compounds are of special interest to petroleum or chemical engineers. Models were based on the eigenvalues of bond connecting-orbital matrix, polarizability effect index (PEI) of alkyl and Pauling's electronegativity. The molecular volume of monosubstituted alkanes RX (X=$NH_2$, OH, SH, F, Cl, Br, I) and alkanes can be correlated by simple linear expressions.

**Results.** Using the model of this paper to estimate the density for RX (see Table 6), the root-mean-square error (rms), the average absolute error and the average relative error are only 0.0208 g/cm$^3$, 0.0171 g/cm$^3$ and 1.85% between the experimental and estimated values respectively.

**Conclusions.** Not only can the models of this paper give very precise calculated results but also have good predictive ability. The models can be used to predict the densities of alkanes and monosubstituted alkanes for whose densities is not measured experimentally yet, which listed in the end of this paper.

**Keywords.** Polarizability effect index PEI; bonding orbital-connecting matrix; molecular volume; density; monoderivatives of hydrocarbon; alkane.

## 1. Introduction

The density of organic compound (especially the density of alkane and monosubstituted alkane) is an important physical property for selecting production facilities in the chemical and petrochemical industries. For example, the data of density is frequently utilized in material accounting and transfer procedure by engineers and it is also one of the major physiochemical properties to be characterized and identified a compound. In addition, densities can be used to predict or estimate other physical properties of compounds such as critical pressures [1, 2]. Unfortunately, several compilations of the experimentally derived density values may not be available for all organic compounds. In many cases it is impractical or impossible to measure the property of interest because insufficient material exists to be tested, there are toxicity issues, or the number of compounds for which data are needed is very large. Thus a reliable means of estimating for engineers would be an advantage. But only few methods to estimate densities from the molecular structures of compounds have been proposed [2, 3, 4]. Karelson [2] and co-workers calculated the molecular volume for liquid organic compound by semi-empirical AM1and then converted the molecular volume to density, which give their model an intrinsic mean of density. Liu [3, 4] even used neural network to predict the density for alkane.

This paper focuses on a practical and rational bond additivity model for evaluating the densities of compounds, which depends on the chemical environment of molecular bonds.

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## 2. Methodology

At a specific temperature, the density of a compound can be expressed as eq 1:

$$D = M/V \tag{1}$$

Where, M is the molecular mass and V denotes the molecular volume. For the alkane RH, we think, its molecular volume can be mainly divided into two parts: i) the contributions of C-C bonds and ii) the contributions of C-H bonds of a molecule. That is,

$$V_{RH} = a_0 + b_0 \Sigma V_{C-C} + c_0 \Sigma V_{C-H} \tag{2}$$

Where $V_{C\text{-}C}$ and $V_{C\text{-}H}$ are the contributions to the volume of each C-C and each C-H bond respectively. Roughly, if the volume of a C-C bond or a C-H bond can be seen as a constant, and the molecular volume may be proportional to the sum of C-C bonds and C-H bonds. In facts, since the chemical environment of C-C bonds in alkane molecule is different from each other, their volume is not a constant. Therefore, taking the simple additivity of number of C-C bond as their volume contributions will raise a large estimating error. So do for the C-H bonds. For a same kind of chemical bond, say C-C or C-H bond, presuming the stronger the bond energy, the shorter the bond length will be, and the smaller the volume will be. Our recent research result [5] shows that not only the chemical environment, but also the bond energies of C-C and C-H bonds can be distinguished and characterized well by the eigenvalues $X_{1CC}$ and $X_{1CH}$ of C-C and C-H bond orbital-connecting matrixes respectively. Thus, it can be leaded to $V_{C\text{-}C} = kX_{1CC}$ and $V_{C\text{-}H} = mX_{1CH}$. Replacing $V_{C\text{-}C}$ and $V_{C\text{-}H}$ with $kX_{1CC}$ and $mX_{1CH}$ in eq 2, we get the eq 3.

$$V_{RH} = a_0 + b_0 \Sigma (kX_{1CC}) + c_0 \Sigma (mX_{1CH}) = a + b\Sigma X_{1CC} + c\Sigma X_{1CH} \tag{3}$$

Where, $X_{1CC}$ and $X_{1CH}$ are the eigenvalues of C-C and C-H bond connecting-matrix respectively, a, b and c are the regression coefficients that can be got by least-square fitting of the data to the experiment values. Combining eq 1 and eq 3, we get,

$$M/D = a + b\Sigma X_{1CC} + c\Sigma X_{1CH} \tag{4}$$

The above equation (eq 4) is expected to estimate molecular volume, and further to calculate the densities of alkanes.

## 3. Calculation of molecular parameters

### 3.1 Polarizability Effect Index (PEI) of alkyl R.

Firstly, cut down a C-C or C-H bond of alkane, we will get two alkyls $R_i$ and $R_j$. The calculation of PEI had been elaborated in literature [6]. According to the literature [6], the PEI values of alkyl $R_i$ and $R_j$ can be calculated easily. Here, for the convenience, the PEI values of some normal alkyls and the increments ΔPEI are cited in Table 1.

**Table 1** The PEI and ΔPEI values of normal alkyl $H(CH_2)_N$

| N | PEI | ΔPEI | N | PEI | ΔPEI |
|---|---|---|---|---|---|
| 1 | 1.0000 | 1.0000 | 6 | 1.2350 | 0.0095 |
| 2 | 1.1405 | 0.1405 | 7 | 1.2414 | 0.0064 |
| 3 | 1.1887 | 0.0481 | 8 | 1.2461 | 0.0047 |
| 4 | 1.2122 | 0.0235 | 9 | 1.2498 | 0.0037 |
| 5 | 1.2260 | 0.0138 | 10 | 1.2527 | 0.0029 |

### 3.2 C-C and C-H σ bonds orbital-connecting matrixes and their eigenvalues

For the convenience of readers, here the calculation of parameters of $\Sigma X_{1CC}$ and $\Sigma X_{1CH}$ [5] for σ bonds were restated briefly. Firstly, using alkyl's polarizability effect index $PEI(R_i)$, $PEI(R_j)$ as the main-diagonal element, 1 as the off-diagonal element, it can be constructed the connecting-matrix $CM_{ij,m}$ for $C_i$-$C_j$ σ bond, and using $PEI(R_i)$, PEI(H) as the main-diagonal element, 1 as the off-diagonal element, it can be constructed the connecting-matrix $CM_{iH,m}$ for $C_i$-H σ bond, respectively. Solving the matrixes, two eigenvalues for each $CM_{ij,m}$ or $CM_{iH,m}$ was got, and the smaller one of each pair of eigenvalues was assigned as $X_{1CC}$ and $X_{1CH}$ respectively. Finally, summing up all $X_{1CC}$ and $X_{1CH}$ of the molecule, the parameters $\Sigma X_{1CC}$ and $\Sigma X_{1CH}$ were obtained respectively.

Taking 2-methyl-2-butane for example to compute the parameters $\Sigma X_{1CC}$ and $\Sigma X_{1CH}$. The calculation procedure of $\Sigma X_{1CC}$ and $\Sigma X_{1CH}$ is listed in Table2 and Table3 respectively.

**Table 2** Calculation of $\Sigma X_{1CC}$ for 2-methylbutane

| $C_i$-$C_j$ bond | $R_i$<br>$PEI(R_i)$ | $R_j$<br>$PEI(R_j)$ | $CM_{ij,m}$ | $X_{1CC}$ (the smaller eigenvalue) | Wt [a] |
|---|---|---|---|---|---|
| $CH_3$—$CH_2CH(CH_3)_2$ | $CH_3$•<br>1.0000 | •$CH_2CH(CH_3)_2$<br>1.2368 | $\begin{bmatrix} 1.0000 & 1 \\ 1 & 1.2368 \end{bmatrix}$ | 0.1114 | 1 |
| $CH_3CH_2$—$CH(CH_3)_2$ | $CH_3CH_2$•<br>1.1405 | •$CH(CH_3)_2$<br>1.2810 | $\begin{bmatrix} 1.1405 & 1 \\ 1 & 1.2810 \end{bmatrix}$ | 0.2083 | 1 |
| $CH_3CH_2CH(CH_3)$–$CH_3$ | $CH_3CH_2\dot{C}HCH_3$<br>1.3292 | •$CH_3$<br>1.0000 | $\begin{bmatrix} 1.3292 & 1 \\ 1 & 1.0000 \end{bmatrix}$ | 0.1511 | 2 |
| $\Sigma X_{1CC}$= 0.1114+0.2083+0.1511+0.1511=0.6219 | | | | | |

[a] Wt denotes the number of a sort of C-C bond in the compound.

**Table 3** Calculation of $\Sigma X_{1CH}$ for 2-methylbutane

| $C_i$-H bond | $R_i$<br>PEI (Ri) | H<br>PEI (H) | $CM_{iH,m}$ | $X_{1CH}$(the smaller eigenvalue ) | Wt [a] |
|---|---|---|---|---|---|
| $CH_3CH_2CH(CH_3)CH_2$–H | $CH_3CH_2CH(CH_3)CH_2$•<br>1.2603 | •H<br>0 | $\begin{bmatrix} 1.2603 & 1 \\ 1 & 0 \end{bmatrix}$ | -0.5518 | 6 |
| $CH_3CH_2(CH_3)_2C$—H | $CH_3CH_2\dot{C}(CH_3)_2$<br>1.4697 | •H<br>0 | $\begin{bmatrix} 1.4697 & 1 \\ 1 & 0 \end{bmatrix}$ | -0.5061 | 1 |
| H–$CH(CH_3)CH(CH_3)_2$ | $CH_3\dot{C}HCH(CH_3)_2$<br>1.3773 | •H<br>0 | $\begin{bmatrix} 1.3773 & 1 \\ 1 & 0 \end{bmatrix}$ | -0.5255 | 2 |
| H–$CH_2CH_2CH(CH_3)_2$ | •$CH_2CH_2CH(CH_3)_2$<br>1.2357 | •H<br>0 | $\begin{bmatrix} 1.2357 & 1 \\ 1 & 0 \end{bmatrix}$ | -0.5576 | 3 |
| $\Sigma X_{1CH}$= -0.5518×6+(-0.5061)+(-0.5255) ×2+(-0.5576) ×3=-6.5407 | | | | | |

[a] Wt denotes the number of a sort of C-H bond in the compound.

Likewise, all the parameter values of $\Sigma X_{1CC}$, $\Sigma X_{1CH}$ for alkanes were calculated and listed in Table 4.

### 4. Regression analysis and discussion

Experimental densities (at 1 atm and 25 $^{o}$C) data [7] are available for 94 alkanes and presented in Table 4. The predictive ability of the following equations was tested on a group of data that was withheld from the existing data set. A random number generator was used to select this predictive set for each of the equations presented.

Eq 5 is the fit to 75 of the 94 alkanes with the remaining 19 withheld as predictive data. Taking experimental densities (at 1 atm and 25 $^{o}$C) of 75 alkanes as data set, using eq 4 as the model, we obtained the eq 5.

$$M_{RH}/D_{RH} = 4.9036 - 12.3752\Sigma X_{1CC} - 18.5263\Sigma X_{1CH} \quad (5)$$

R=0.9935□S=2.72□n=75□F=2722.60

The result of this two-parameter equation is very good; its correlation coefficient is 0.9935. Using eq 5 to estimate the density for these 75 alkanes, the root-mean-square error (rms) is only 0.0111 g/cm$^3$ between the experimental and estimated values. The rms=$[(D_{exp.}\square D_{calc.})^2/(n\square 1)]^{1/2}$, in which n is the number of examined compounds. Table 5 illustrates the predictive ability of eq 5 for the given set of 19 withheld alkanes. The eq 5 has a very good predictive ability, and the root-mean-square error (rms) is only 0.00935 g/cm$^3$ between the experimental and predicted values. So eq 5 is recommended to predict the density of alkanes.

The density of alkane can be estimated well, then how to estimate that of monosubsituted alkane? When a hydrogen atom in alkane RH is replaced by a substituent X (X designated halogen or other functional groups), the monosubstituted alkane molecule RX will generate. Comparing the two series of compounds, it can be found there are two primary discrepancy between compounds RH and RX: i) A C-H bond in alkane has changed into the corresponding C-X bond of RX; ii) Generally speaking, an alkane molecule RH is nonpolar, while RX belongs to the polar molecule. If taking the alkane RH as unperturbed system and the monosubstituted alkane RX as the corresponding perturbed system, one can estimate the molecular volume $V_{RX}$ for the perturbed system RX with eq 6.

$$V_{RX} = V_{RH} + \Delta\Delta V + V_X \quad (6)$$

Where, $V_{RH}$ is the molecular volume of unperturbed system RH; $\Delta\Delta V$ designates the volume increments of the alkyl R from RH to RX system, which is caused by the H atom changing into the substituent X; $V_X$ is the volume of the substituent X, which can be scaled approximately by the atomic radii ($r_X$) of the atom attached directly to the alkyl R. The volume increments $\Delta\Delta V$ is the difference between the volume of alkyl R in the nonpolar molecule RH and the volume of alkyl R in the polar one RX, which, we think, can be correlated with the polarizability of alkyl R and the electronegativity of group X. Based on the above analysis, we suggest a single expression (eq 7) to evaluate the molecular volumes and further to calculate the densities for different series of monosubstituted alkane RX.

$$M_{RX}/D_{RX} = a + br_X + cPEI + dPEI \times \chi_X + e\Sigma X_{1CC} + f\Sigma X_{1CH} \quad (7)$$

Where, $r_x$ and $\chi_x$ are the atomic radii [8] and electronegativity (Pauling scale) of the atom attached directly to the alkyl R respectively. PEI is the polarizability effect index of alkyl R in RX. $\Sigma X_{1CC}$ and $\Sigma X_{1CH}$ is the sum of eigenvalues of matrixes $CM_{ij,m}$ and $CM_{iH,m}$ for C-C and C-H bonds in alkyl R respectively.

Now, take 2-bromo-2-methylbutane for example to show how to calculate $\Sigma X_{1CC}$ and $\Sigma X_{1CH}$ for RX. At first, the bromine atom was replaced with hydrogen atom, that is, $(CH_3)_2CBrCH_2CH_3$ was returned to $(CH_3)_2CHCH_2CH_3$. Then the connecting-matrix $CM_{ij,m}$ and $CM_{iH,m}$ were constructed as the 2-methylbutane (see Table 1 and Table 2), and the $X_{1CC}$ and $X_{1CH}$ values, 0.6219 and -6.5407 were obtained respectively. Since having the same σ carbon-carbon bond skeletons, monosubstituted alkane $(CH_3)_2CBrCH_2CH_3$ has the equal $\Sigma X_{1CC}$ value as that of alkane $(CH_3)_2CHCH_2CH_3$, that is, its $\Sigma X_{1CC}$=0.6219. But comparing with $(CH_3)_2CHCH_2CH_3$, the 2-bromo-2-methylbutane $(CH_3)_2CBrCH_2CH_3$ loses one C-H bonds which is bond $Et(Me)_2C$-H, so the $\Sigma X_{1CH}$ value of 2-bromo-2-methylbutane must cut out the $X_{1CH}$ values of the lost C-H bond. That is, its

$\Sigma X_{1CH}$=(-0.5518×6+(-0.5061)+(-0.5255) ×2+(-0.5576) ×3)-(-0.5061)=-6.5407-(-0.5061)=-6.0346. Likewise, all the parameter values of $\Sigma X_{1CC}$, $\Sigma X_{1CH}$ for monosubstituted alkanes were calculated and listed in Table 6.

**Table 4** Experimental Density values (at 1 atm and 25 $^{o}$C) for 94 Alkanes

| no | RH [a] | $\Sigma X_{1CC}$ | $\Sigma X_{1CH}$ | D $_{exp.}$□g.cm$^{-3}$□ | no | RH[a] | $\Sigma X_{1CC}$ | $\Sigma X_{1CH}$ | $D_{exp.}$□g.cm$^{-3}$□ |
|---|---|---|---|---|---|---|---|---|---|
| 1 | C3 | 0.1356 | -4.5074 | 0.4930 | 48 | 235mmmC7 | 2.1672 | -11.5210 | 0.7413 |
| 2 | C4 | 0.3203 | -5.5244 | 0.5730 | 49 | 236mmmC7 | 2.1216 | -11.5287 | 0.7305 |
| 3 | 2mC3 | 0.3921 | -5.5327 | 0.5510 | 50 | 244mmmC7 | 2.2480 | -11.5188 | 0.7308 |
| 4 | 22mmC3 | 0.7552 | -6.5532 | 0.5852 | 51 | 245mmmC7 | 2.1754 | -11.5197 | 0.7373 |
| 5 | C6 | 0.7533 | -7.5404 | 0.6548 | 52 | 246mmmC7 | 2.1189 | -11.5273 | 0.7190 |
| 6 | 2mC5 | 0.8540 | -7.5453 | 0.6500 | 53 | 255mmmC7 | 2.2158 | -11.5259 | 0.7362 |
| 7 | 3mC5 | 0.8753 | -7.5440 | 0.6598 | 54 | 334mmmC7 | 2.2176 | -11.5110 | 0.7527 |
| 8 | 22mmC4 | 1.0264 | -7.5706 | 0.6444 | 55 | 344mmmC7 | 2.3170 | -11.5096 | 0.7535 |
| 9 | C8 | 1.2266 | -9.5424 | 0.6986 | 56 | 345mmmC7 | 2.2352 | -11.5108 | 0.7519 |
| 10 | 23mmC6 | 1.4990 | -9.5407 | 0.6912 | 57 | 3e2mC7 | 2.0741 | -11.5162 | 0.7398 |
| 11 | 24mmC6 | 1.4798 | -9.5432 | 0.6962 | 58 | 4e2mC7 | 2.0602 | -11.5178 | 0.7322 |
| 12 | 25mmC6 | 1.4418 | -9.5482 | 0.6901 | 59 | 5e2mC7 | 2.0346 | -11.5237 | 0.7318 |
| 13 | 34mmC6 | 1.5284 | -9.5370 | 0.7151 | 60 | 3e3mC7 | 2.1826 | -11.5132 | 0.7463 |
| 14 | 224mmmC5 | 1.6445 | -9.5487 | 0.6877 | 61 | 4e3mC7 | 2.1204 | -11.5095 | 0.7466 |
| 15 | 2mC8 | 1.5800 | -10.5423 | 0.7095 | 62 | 5e3mC7 | 2.0804 | -11.5952 | 0.7368 |
| 16 | 3mC8 | 1.6165 | -10.5373 | 0.7170 | 63 | 3e4mC7 | 2.1159 | -11.5106 | 0.7468 |
| 17 | 4mc8 | 1.6299 | -10.5432 | 0.7160 | 64 | 4e4mC7 | 2.2037 | -11.5087 | 0.7472 |
| 18 | 24mmC7 | 1.7439 | -10.5347 | 0.7115 | 65 | 4PrC7 | 1.9584 | -11.5144 | 0.7321 |
| 19 | 3eC7 | 1.6668 | -10.5296 | 0.7225 | 66 | 4iPrC7 | 2.0915 | -11.7131 | 0.7354 |
| 20 | 4eC7 | 1.6803 | -10.5265 | 0.7241 | 67 | 2233mmmmC6 | 2.5074 | -11.5088 | 0.7609 |
| 21 | 223mmmC6 | 1.9732 | -10.5326 | 0.7257 | 68 | 2234mmmmC6 | 2.4178 | -11.5119 | 0.7513 |
| 22 | 233mmmC6 | 2.0003 | -10.5284 | 0.7345 | 69 | 2235mmmmC6 | 2.3552 | -11.5217 | 0.7336 |
| 23 | 234mmmC6 | 1.9256 | -10.5280 | 0.7354 | 70 | 2244mmmmC6 | 2.4382 | -11.5202 | 0.7424 |
| 24 | 244mmmC6 | 1.9640 | -10.5333 | 0.7201 | 71 | 2245mmmmC6 | 2.3378 | -11.5244 | 0.7316 |
| 25 | 334mmmC6 | 2.0291 | -10.5253 | 0.7414 | 72 | 2255mmmmC6 | 2.3523 | -11.5340 | 0.7148 |
| 26 | 2m4eC6 | 1.7826 | -10.5409 | 0.7195 | 73 | 2334mmmmC6 | 2.4615 | -11.5143 | 0.7656 |
| 27 | 3m3eC6 | 1.9151 | -10.5239 | 0.7371 | 74 | 2335mmmmC6 | 2.3895 | -11.5158 | 0.7449 |
| 28 | 2233mmmmC5 | 2.2165 | -10.5260 | 0.7530 | 75 | 2344mmmmC6 | 2.4442 | -11.5083 | 0.7586 |
| 29 | 23mm3eC5 | 2.0373 | -10.5208 | 0.7508 | 76 | 2345mmmmC6 | 2.3348 | -11.5124 | 0.7456 |
| 30 | 22mmC8 | 2.0324 | -11.5370 | 0.7208 | 77 | 3344mmmmC6 | 2.5621 | -11.5018 | 0.7789 |
| 31 | 24mmC8 | 2.0018 | -11.5368 | 0.7226 | 78 | 22mm3eC6 | 2.2189 | -11.5105 | 0.7447 |
| 32 | 25mmC8 | 1.9952 | -11.5282 | 0.7264 | 79 | 23mm3eC6 | 2.3488 | -11.5047 | 0.7599 |
| 33 | 27mmC8 | 1.9391 | -11.5382 | 0.7202 | 80 | 23mm4eC6 | 2.2483 | -11.5085 | 0.7516 |
| 34 | 33mmC8 | 2.1024 | -11.5263 | 0.7351 | 81 | 24mm3eC6 | 2.2569 | -11.5071 | 0.7514 |
| 35 | 34mmC8 | 2.0581 | -11.5196 | 0.7410 | 82 | 24mm4eC6 | 2.3046 | -11.5116 | 0.7525 |
| 36 | 35mmC8 | 2.0393 | -11.5221 | 0.7329 | 83 | 25mm3eC6 | 2.1932 | -11.5159 | 0.7368 |
| 37 | 36mmC8 | 2.0185 | -11.5266 | 0.7324 | 84 | 33mm4eC6 | 2.3590 | -11.5038 | 0.7598 |
| 38 | 44mmC8 | 2.1275 | -11.5196 | 0.7312 | 85 | 34mm3eC6 | 2.3772 | -11.5016 | 0.7596 |
| 39 | 45mmC8 | 2.0709 | -11.5168 | 0.7432 | 86 | 33eeC6 | 2.2645 | -11.5010 | 0.7575 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 40 | 3eC8 | 1.9220 | -11.5227 | 0.7359 | 87 | 34eeC6 | 2.1626 | -11.3856 | 0.7472 |
| 41 | 4eC8 | 1.9423 | -11.5178 | 0.7343 | 88 | 2m3ipC6 | 2.2279 | -11.5102 | 0.7436 |
| 42 | 223mmmC7 | 2.2363 | -11.5382 | 0.7385 | 89 | 22334mmmmmC5 | 2.6542 | -11.3029 | 0.7767 |
| 43 | 224mmmC7 | 2.2090 | -11.5255 | 0.7237 | 90 | 22344mmmmmC5 | 2.6037 | -11.5120 | 0.7636 |
| 44 | 225mmmC7 | 2.1848 | -11.5308 | 0.7243 | 91 | 223mmm3eC5 | 2.5709 | -11.4998 | 0.7780 |
| 45 | 226mmmC7 | 2.1431 | -11.5376 | 0.7200 | 92 | 234mmm3eC5 | 2.4966 | -11.4999 | 0.7735 |
| 46 | 233mmmC7 | 2.2674 | -11.5794 | 0.7450 | 93 | 2m33eeC5 | 2.4130 | -11.4958 | 0.7755 |
| 47 | 234mmmC7 | 2.2022 | -11.5152 | 0.7447 | 94 | 24mm3ipC5 | 2.3679 | -11.5060 | 0.7545 |

[a] m, methyl; e, ethyl; for example 2mmC3 represent 2,2-dimethyl-propane.

**Table 5** Predictive Ability of equation 5

| no | RH | $D_{exp.}$□g·cm$^{-3}$□$D_{calc.}$□g·cm$^{-3}$□ | | Δ | no | RH | $D_{exp.}$□g·cm$^{-3}$□$D_{calc.}$□g·cm$^{-3}$□ | | Δ |
|---|---|---|---|---|---|---|---|---|---|
| 9 | C8 | 0.6986 | 0.6846 | 0.0140 | 42 | 223mmmC7 | 0.7385 | 0.7435 | -0.0050 |
| 10 | 23mmC6 | 0.6912 | 0.6989 | -0.0077 | 45 | 226mmmC7 | 0.7200 | 0.7391 | -0.0191 |
| 12 | 25mmC6 | 0.6901 | 0.6953 | -0.0052 | 50 | 244mmmC7 | 0.7308 | 0.7455 | -0.0147 |
| 14 | 224mmmC5 | 0.6877 | 0.7061 | -0.0184 | 51 | 245mmmC7 | 0.7373 | 0.7419 | -0.0046 |
| 21 | 223mmmC6 | 0.7257 | 0.7289 | -0.0032 | 55 | 344mmmC7 | 0.7535 | 0.7495 | 0.0040 |
| 22 | 233mmmC6 | 0.7345 | 0.7306 | 0.0039 | 62 | 5e3mC7 | 0.7368 | 0.7321 | 0.0047 |
| 25 | 334mmmC6 | 0.7414 | 0.7323 | 0.0091 | 78 | 22mm3eC6 | 0.7447 | 0.7447 | 0.0000 |
| 28 | 2233mmmmC5 | 0.753 | 0.7421 | 0.0109 | 85 | 34mm3eC6 | 0.7596 | 0.7530 | 0.0066 |
| 34 | 33mmC8 | 0.7351 | 0.7379 | -0.0028 | 94 | 24mm3ipC5 | 0.7545 | 0.7523 | 0.0022 |
| 36 | 35mmC8 | 0.7329 | 0.7353 | -0.0024 | | | | | |

Taking some measured densities [7] (at 1 atm and 20 $^{o}$C) of various monosubsituted alkanes RX as data set (listed in Table 6), using eq 7 as the model, we obtained the following correlation expression.

$$M/D = 0.7428 + 20.0722 r_X + 16.1654 PEI - 5.1047 PEI \times \chi_X - 7.6872 \Sigma X_{1CC} - 17.9039 \Sigma X_{1CH} \quad (8)$$

R=0.9949□S=3.09□n=213□F=4042.69

For the data set including 213 compounds RX (X= NH2, OH, SH, F, Cl, Br, I) and the density range from 0.6 to 2.3 g/cm$^3$, the correlation coefficient is excellence (R=0.9949). Using eq 8 to estimate the density for RX (see Table 6), the root-mean-square error (rms), the average absolute error and the average relative error are only 0.0208 g/cm$^3$, 0.0171 g/cm$^3$ and 1.85% between the experimental and estimated values respectively. Figure 1 shows the plot of experimental density versus calculated ones (determined by eq 8) of monosubstituted alkane. The straight line represents an exact prediction. From Table 6 and Figure 1, one can see that the estimated density agrees with experimental ones very well.

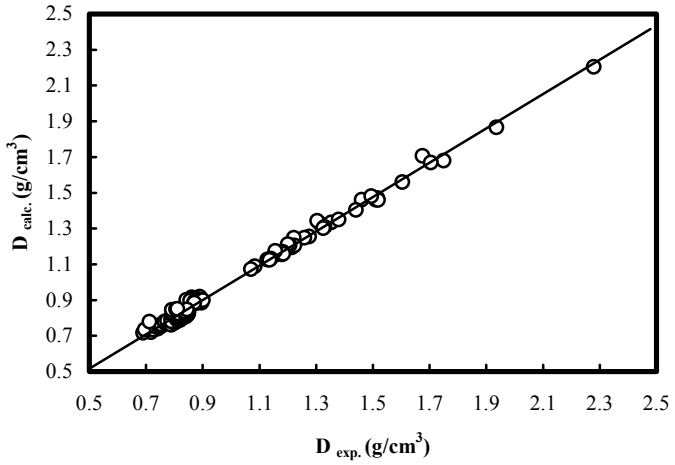


**Fig. 1** The plot of calculated (by eq 8) vs. experimental density of monosubstituted alkane RX

The stability of the eq 8 was tested on a group of data that was withheld from the existing data set. Eq 9 is the fit to 173 of the 213 monosubstituted alkanes with the remaining 40 withheld as predictive data. Taking experimental densities (at 1 atm and 20 $^{o}$C) of 173 monosubstituted alkanes as data set, using eq 7 as the model, we obtained the eq 9.

$$M/D = -0.4332 + 19.4789 r_X + 18.8429 PEI - 5.6175 PEI \times \chi_X - 8.2804 \Sigma X_{1CC} - 18.0114 \Sigma X_{1CH} \quad (9)$$

R=0.9949□S=3.07□n=173□F=3264.56

Table 7 illustrates the predictive ability of eq 9 for the given set of 40 withheld monosubstituted alkanes. The eq 9 has a very good predictive ability, the root-mean-square error (rms) and the average absolute error are only 0.0232 g/cm$^3$ and 0.0177 g/cm$^3$ between the experimental and predicted values determined by eq 9. For the same 40 monosubstituted alkanes, the average absolute error is 0.0178 g/cm$^3$ between the experimental and the estimated values determined by eq 8. It shows that eq 8 is a stable model for predicting the density of RX.

Not only can eq 8 give a very satisfying result, but also each item of eq 8 has a very explicit physical meaning. In our previous work[5], we have demonstrated that $X_{1CC}$ and $X_{1CH}$ correlate with the energy of C-C and C-H bond of a molecule, respectively. As we know, there is a proportion by inversion between bond energy and bond length for a same sort of bond, i.e. the lower is the bond energy, the longer is the bond length for the same sort of bond. Thus, in view of this point, the eigenvalues of orbital-connecting matrix $\Sigma X_{1CC}$ and $\Sigma X_{1CH}$ represent the contributions of all C-C and C-H bonds of a molecule to the molecular volume; $r_X$ scales the contribution of substituent X to the volume of a molecule. The larger $r_X$, and the longer C-X bond, will result in a larger contribution to the molecular volume. For the two items PEI×$\chi_x$ and PEI, its physical meaning can be explained as following: Distribution of the electronic cloud of C-C and C-H will be changed and result in the stretch of C-C and C-H bonds when a hydrogen atom of nonpolar alkane is replaced with a polar substituent X, which will result in the volume change of alkyl R eventually. That is to say, PEI×$\chi_x$ together with PEI contributes the perturbation volume ΔΔV from RH to RX system, which is caused by the H atom changing into the substituent X.

**Table 6** Experimental and Estimated Density (at 1 atm and 20 °C) f or 213 Monosubstituted Alkanes

| no | RX [a] | PEI | $r_x$ [b] | $\Sigma X_{1CC}$ | $\Sigma X_{1CH}$ | D exp. ($g \cdot cm^{-3}$) | D calc. [c] ($g \cdot cm^{-3}$) | $\Delta$ [d] |
|---|---|---|---|---|---|---|---|---|
| 1 | PrNH2 | 1.1887 | 0.54 | 0.1356 | -3.9385 | 0.7173 | 0.7211 | -0.0038 |
| 2 | i-PrNH2 | 1.2810 | 0.54 | 0.1356 | -3.9604 | 0.6891 | 0.7171 | -0.0280 |
| 3 | n-BuNH2 | 1.2122 | 0.54 | 0.3203 | -4.9612 | 0.7414 | 0.7394 | 0.0020 |
| 4 | s-BuNH2 | 1.3292 | 0.54 | 0.3203 | -4.9881 | 0.7246 | 0.7352 | -0.0106 |
| 5 | t-BuNH2 | 1.4215 | 0.54 | 0.3921 | -5.0166 | 0.6958 | 0.7351 | -0.0393 |
| 6 | C5NH2 | 1.2260 | 0.54 | 0.5296 | -5.9741 | 0.7544 | 0.7548 | -0.0004 |
| 7 | 2NC5 | 1.3527 | 0.54 | 0.5296 | -6.0031 | 0.7348 | 0.7509 | -0.0161 |
| 8 | 3NC5 | 1.3773 | 0.54 | 0.5296 | -6.0085 | 0.7487 | 0.7501 | -0.0014 |
| 9 | 3mNC4 | 1.2357 | 0.54 | 0.6219 | -5.9831 | 0.7505 | 0.7584 | -0.0079 |
| 10 | NC6 | 1.2350 | 0.54 | 0.7533 | -6.9826 | 0.7660 | 0.7674 | -0.0014 |
| 11 | 2NC6 | 1.3665 | 0.54 | 0.7533 | -7.0125 | 0.7533 | 0.7638 | -0.0105 |
| 12 | 3mNC5 | 1.2495 | 0.54 | 0.8753 | -6.9896 | 0.7670 | 0.7722 | -0.0052 |
| 13 | 33mm2NC4 | 1.4254 | 0.54 | 1.0264 | -7.0553 | 0.7688 | 0.7714 | -0.0026 |
| 14 | NC7 | 1.2414 | 0.54 | 0.9866 | -7.9861 | 0.7754 | 0.7782 | -0.0028 |
| 15 | 4NC7 | 1.4243 | 0.54 | 0.9866 | -8.0269 | 0.7670 | 0.7737 | -0.0067 |
| 16 | 4mNC6 | 1.2488 | 0.54 | 1.1214 | -7.9889 | 0.7802 | 0.7834 | -0.0032 |
| 17 | 4m2NC6 | 1.3900 | 0.54 | 1.1214 | -8.0206 | 0.7655 | 0.7799 | -0.0144 |
| 18 | 24mm2NC5 | 1.5167 | 0.54 | 1.1998 | -8.0519 | 0.7119 | 0.7797 | -0.0678 |
| 19 | NC8 | 1.2461 | 0.54 | 1.2266 | -8.9872 | 0.7826 | 0.7872 | -0.0046 |
| 20 | 2NC8 | 1.3819 | 0.54 | 1.2266 | -9.0179 | 0.7744 | 0.7842 | -0.0098 |
| 21 | NC9 | 1.2498 | 0.54 | 1.4718 | -9.9849 | 0.7886 | 0.7951 | -0.0065 |
| 22 | MeOH | 1.0000 | 0.46 | 0.0000 | -1.8540 | 0.7914 | 0.7660 | 0.0254 |
| 23 | EtOH | 1.1405 | 0.46 | 0.0000 | -2.9045 | 0.7893 | 0.7618 | 0.0275 |
| 24 | PrOH | 1.1887 | 0.46 | 0.1356 | -3.9385 | 0.7997 | 0.7713 | 0.0284 |
| 25 | n-BuOH | 1.2122 | 0.46 | 0.3203 | -4.9612 | 0.8098 | 0.7818 | 0.0280 |
| 26 | s-BuOH | 1.3292 | 0.46 | 0.3203 | -4.9881 | 0.8063 | 0.7792 | 0.0271 |
| 27 | i-BuOH | 1.2368 | 0.46 | 0.3921 | -4.9753 | 0.8018 | 0.7846 | 0.0172 |
| 28 | t-BuOH | 1.4215 | 0.46 | 0.3921 | -5.0166 | 0.7887 | 0.7806 | 0.0081 |
| 29 | C5OH | 1.2260 | 0.46 | 0.5296 | -5.9741 | 0.8144 | 0.7917 | 0.0227 |
| 30 | 2OHC5 | 1.3527 | 0.46 | 0.5296 | -6.0031 | 0.8094 | 0.7893 | 0.0201 |
| 31 | 3OHC5 | 1.3773 | 0.46 | 0.5296 | -6.0085 | 0.8203 | 0.7888 | 0.0315 |
| 32 | 22mm1OHC3 | 1.2849 | 0.46 | 0.7552 | -6.0071 | 0.8120 | 0.8005 | 0.0115 |
| 33 | 3mOHC4 | 1.2357 | 0.46 | 0.6219 | -5.9831 | 0.8104 | 0.7957 | 0.0147 |
| 34 | 2m2OHC4 | 1.4697 | 0.46 | 0.6219 | -6.0346 | 0.8096 | 0.7915 | 0.0181 |
| 35 | 3m2OHC4 | 1.3773 | 0.46 | 0.6219 | -6.0152 | 0.8180 | 0.7930 | 0.0250 |
| 36 | OHC6 | 1.2350 | 0.46 | 0.7533 | -6.9826 | 0.8136 | 0.8001 | 0.0135 |
| 37 | 2OHC6 | 1.3665 | 0.46 | 0.7533 | -7.0125 | 0.8159 | 0.7979 | 0.0180 |
| 38 | 2mOHC5 | 1.2741 | 0.46 | 0.8540 | -6.9967 | 0.8263 | 0.8038 | 0.0225 |
| 39 | 3mOHC5 | 1.2495 | 0.46 | 0.8753 | -6.9896 | 0.8242 | 0.8054 | 0.0188 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 40 | 4mOHC5 | 1.2398 | 0.46 | 0.8540 | -6.9886 | 0.8131 | 0.8044 | 0.0087 |
| 41 | 3m2OHC5 | 1.4008 | 0.46 | 0.8753 | -7.0235 | 0.8307 | 0.8029 | 0.0278 |
| 42 | 4m2OHC5 | 1.3762 | 0.46 | 0.8540 | -7.0195 | 0.8075 | 0.8021 | 0.0054 |
| 43 | 2m3OHC5 | 1.4254 | 0.46 | 0.8540 | -7.0300 | 0.8243 | 0.8013 | 0.0230 |
| 44 | 3m3OHC5 | 1.5178 | 0.46 | 0.8753 | -7.0476 | 0.8286 | 0.8012 | 0.0274 |
| 45 | 22mmOHC4 | 1.3084 | 0.46 | 1.0264 | -7.0298 | 0.8283 | 0.8087 | 0.0196 |
| 46 | 23mmOHC4 | 1.2838 | 0.46 | 0.9654 | -7.0005 | 0.8297 | 0.8089 | 0.0208 |
| 47 | 23mm2OHC4 | 1.5178 | 0.46 | 0.9654 | -7.0532 | 0.8236 | 0.8049 | 0.0187 |
| 48 | 2eOHC4 | 1.2838 | 0.46 | 0.8753 | -6.9976 | 0.8326 | 0.8048 | 0.0278 |
| 49 | OHC7 | 1.2414 | 0.46 | 0.9866 | -7.9861 | 0.8219 | 0.8076 | 0.0143 |
| 50 | 2OHC7 | 1.3755 | 0.46 | 0.9866 | -8.0165 | 0.8167 | 0.8056 | 0.0111 |
| 51 | 4OHC7 | 1.4243 | 0.46 | 0.9866 | -8.0269 | 0.8183 | 0.8049 | 0.0134 |
| 52 | 2mOHC6 | 1.2831 | 0.46 | 1.0914 | -8.0003 | 0.8270 | 0.8110 | 0.0160 |
| 53 | 3mOHC6 | 1.2585 | 0.46 | 1.1214 | -7.9911 | 0.8258 | 0.8131 | 0.0127 |
| 54 | 4mOHC6 | 1.2488 | 0.46 | 1.1214 | -7.9889 | 0.8239 | 0.8132 | 0.0107 |
| 55 | 5mOHC6 | 1.2440 | 0.46 | 1.0914 | -7.9912 | 0.8119 | 0.8116 | 0.0003 |
| 56 | 2m2OHC6 | 1.5070 | 0.46 | 1.0914 | -8.0483 | 0.8119 | 0.8079 | 0.0040 |
| 57 | 5m2OHC6 | 1.3803 | 0.46 | 1.0914 | -8.0220 | 0.8140 | 0.8096 | 0.0044 |
| 58 | 2m3OHC6 | 1.4489 | 0.46 | 1.0914 | -8.0365 | 0.8407 | 0.8086 | 0.0321 |
| 59 | 3m3OHC6 | 1.5413 | 0.46 | 1.1214 | -8.0516 | 0.8233 | 0.8091 | 0.0142 |
| 60 | 5m3OHC6 | 1.4243 | 0.46 | 1.0914 | -8.0314 | 0.8270 | 0.8090 | 0.0180 |
| 61 | 24mmOHC5 | 1.2879 | 0.46 | 1.1998 | -8.0032 | 0.7930 | 0.8155 | -0.0225 |
| 62 | 24mm2OHC5 | 1.5167 | 0.46 | 1.1998 | -8.0519 | 0.8103 | 0.8123 | -0.0020 |
| 63 | 22mm3OHC5 | 1.4735 | 0.46 | 1.2794 | -8.0462 | 0.8253 | 0.8161 | 0.0092 |
| 64 | 24mm3OHC5 | 1.4735 | 0.46 | 1.1998 | -8.0433 | 0.8288 | 0.8129 | 0.0159 |
| 65 | 2OHC8 | 1.3819 | 0.46 | 1.2266 | -9.0179 | 0.8193 | 0.8121 | 0.0072 |
| 66 | 3OHC8 | 1.4236 | 0.46 | 1.2266 | -9.0267 | 0.8258 | 0.8116 | 0.0142 |
| 67 | 4OHC8 | 1.4381 | 0.46 | 1.2266 | -9.0298 | 0.8186 | 0.8114 | 0.0072 |
| 68 | 6m2OHC7 | 1.3845 | 0.46 | 1.3335 | -9.0214 | 0.8218 | 0.8160 | 0.0058 |
| 69 | 2m3OHC7 | 1.4627 | 0.46 | 1.3335 | -9.0379 | 0.8235 | 0.8151 | 0.0084 |
| 70 | 4m4OHC7 | 1.5648 | 0.46 | 1.3765 | -9.0519 | 0.8248 | 0.8162 | 0.0086 |
| 71 | 25mmOHC6 | 1.2921 | 0.46 | 1.4418 | -9.0037 | 0.8280 | 0.8213 | 0.0067 |
| 72 | 23mm2OHC6 | 1.5551 | 0.46 | 1.4990 | -9.0515 | 0.8365 | 0.8210 | 0.0155 |
| 73 | 25mm2OHC6 | 1.5208 | 0.46 | 1.4418 | -9.0523 | 0.8227 | 0.8184 | 0.0043 |
| 74 | 22mm3OHC6 | 1.4970 | 0.46 | 1.5296 | -9.0474 | 0.8342 | 0.8222 | 0.0120 |
| 75 | 25mm3OHC6 | 1.4724 | 0.46 | 1.4418 | -9.0426 | 0.8212 | 0.8190 | 0.0022 |
| 76 | 35mm3OHC6 | 1.5648 | 0.46 | 1.4798 | -9.0559 | 0.8373 | 0.8199 | 0.0174 |
| 77 | 44mm3OHC6 | 1.4970 | 0.46 | 1.5865 | -9.0399 | 0.8341 | 0.8252 | 0.0089 |
| 78 | 2eOHC6 | 1.3066 | 0.46 | 1.3679 | -9.0002 | 0.8319 | 0.8188 | 0.0131 |
| 79 | 3e3OHC6 | 1.5894 | 0.46 | 1.4112 | -9.0524 | 0.8373 | 0.8177 | 0.0196 |
| 80 | 244mmm2OHC5 | 1.5402 | 0.46 | 1.6445 | -9.0566 | 0.8225 | 0.8263 | -0.0038 |
| 81 | 224mmm3OHC5 | 1.5216 | 0.46 | 1.6445 | -9.0530 | 0.8297 | 0.8265 | 0.0032 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 82 | 234mmm3OHC5 | 1.6140 | 0.46 | 1.6247 | -9.0629 | 0.8492 | 0.8254 | 0.0238 |
| 83 | 3e2m2OHC5 | 1.5648 | 0.46 | 1.5374 | -9.0484 | 0.8382 | 0.8229 | 0.0153 |
| 84 | 3e2m3OHC5 | 1.6140 | 0.46 | 1.5374 | -9.0577 | 0.8280 | 0.8224 | 0.0056 |
| 85 | OHC9 | 1.2498 | 0.46 | 1.4718 | -9.9849 | 0.8273 | 0.8196 | 0.0077 |
| 86 | 2OHC9 | 1.3866 | 0.46 | 1.4718 | -10.0157 | 0.8471 | 0.8180 | 0.0291 |
| 87 | 3OHC9 | 1.4300 | 0.46 | 1.4718 | -10.0249 | 0.8250 | 0.8175 | 0.0075 |
| 88 | 4OHC9 | 1.4471 | 0.46 | 1.4718 | -10.0285 | 0.8282 | 0.8173 | 0.0109 |
| 89 | 5OHC9 | 1.4519 | 0.46 | 1.4718 | -10.0295 | 0.8356 | 0.8172 | 0.0184 |
| 90 | 2m2OHC8 | 1.5224 | 0.46 | 1.5800 | -10.0467 | 0.8210 | 0.8201 | 0.0009 |
| 91 | 4m4OHC8 | 1.5786 | 0.46 | 1.6299 | -10.0496 | 0.8267 | 0.8220 | 0.0047 |
| 92 | 26mm2OHC7 | 1.5250 | 0.46 | 1.8132 | -10.0486 | 0.8186 | 0.8284 | -0.0098 |
| 93 | 23mm3OHC7 | 1.6032 | 0.46 | 1.7312 | -10.0541 | 0.8395 | 0.8255 | 0.0140 |
| 94 | 26mm3OHC7 | 1.4765 | 0.46 | 1.8132 | -10.0389 | 0.8212 | 0.8290 | -0.0078 |
| 95 | 24mm4OHC7 | 1.5883 | 0.46 | 1.7439 | -10.0519 | 0.8215 | 0.8261 | -0.0046 |
| 96 | 26mm4OHC7 | 1.4713 | 0.46 | 1.8132 | -10.0378 | 0.8114 | 0.8290 | -0.0176 |
| 97 | 4e4OHC7 | 1.6129 | 0.46 | 1.6803 | -10.0483 | 0.8350 | 0.8242 | 0.0108 |
| 98 | 2e3mOHC6 | 1.3301 | 0.46 | 1.7963 | -9.9929 | 0.8486 | 0.8313 | 0.0173 |
| 99 | 223mmm3OHC6 | 1.6375 | 0.46 | 1.9732 | -10.0589 | 0.8474 | 0.8342 | 0.0132 |
| 100 | 244mmm3OHC6 | 1.5451 | 0.46 | 1.9640 | -10.0422 | 0.8489 | 0.8347 | 0.0142 |
| 101 | OHC10 | 1.2527 | 0.46 | 1.7204 | -10.9812 | 0.8297 | 0.8246 | 0.0051 |
| 102 | 2OHC10 | 1.3903 | 0.46 | 1.7204 | -11.0121 | 0.8250 | 0.8230 | 0.0020 |
| 103 | 4OHC10 | 1.4535 | 0.46 | 1.7204 | -11.0254 | 0.8261 | 0.8224 | 0.0037 |
| 104 | 27mm3OHC8 | 1.4807 | 0.46 | 1.9391 | -11.0344 | 0.8152 | 0.8291 | -0.0139 |
| 105 | 26mm4OHC8 | 1.4851 | 0.46 | 1.9780 | -11.0300 | 0.8114 | 0.8308 | -0.0194 |
| 106 | 3e2m3OHC7 | 1.6513 | 0.46 | 2.0741 | -11.0451 | 0.8455 | 0.8339 | 0.0116 |
| 107 | MeBr | 1.0000 | 1.03 | 0.0000 | -1.8540 | 1.6755 | 1.7066 | -0.0311 |
| 108 | EtBr | 1.1405 | 1.03 | 0.0000 | -2.9045 | 1.4604 | 1.4607 | -0.0003 |
| 109 | PrBr | 1.1887 | 1.03 | 0.1356 | -3.9385 | 1.3537 | 1.3349 | 0.0188 |
| 110 | i-PrBr | 1.2810 | 1.03 | 0.1356 | -3.9604 | 1.3140 | 1.3278 | -0.0138 |
| 111 | n-BuBr | 1.2122 | 1.03 | 0.3203 | -4.9612 | 1.2758 | 1.2562 | 0.0196 |
| 112 | s-BuBr | 1.3292 | 1.03 | 0.3203 | -4.9881 | 1.2585 | 1.2493 | 0.0092 |
| 113 | t-BuBr | 1.4215 | 1.03 | 0.3921 | -5.0166 | 1.2209 | 1.2486 | -0.0277 |
| 114 | n-C5Br | 1.2260 | 1.03 | 0.5296 | -5.9741 | 1.2182 | 1.2022 | 0.0160 |
| 115 | 2BrC5 | 1.3527 | 1.03 | 0.5296 | -6.0031 | 1.2075 | 1.1960 | 0.0115 |
| 116 | 3BrC5 | 1.3773 | 1.03 | 0.5296 | -6.0085 | 1.2140 | 1.1949 | 0.0191 |
| 117 | 2m1BrC4 | 1.2603 | 1.03 | 0.6219 | -5.9889 | 1.2234 | 1.2062 | 0.0172 |
| 118 | 3m1BrC4 | 1.2357 | 1.03 | 0.6219 | -5.9831 | 1.2071 | 1.2074 | -0.0003 |
| 119 | 22mm1BrC3 | 1.2849 | 1.03 | 0.7552 | -6.0071 | 1.1997 | 1.2127 | -0.0130 |
| 120 | C6Br | 1.2350 | 1.03 | 0.7533 | -6.9826 | 1.1744 | 1.1624 | 0.0120 |
| 121 | 2BrC6 | 1.3665 | 1.03 | 0.7533 | -7.0125 | 1.1658 | 1.1569 | 0.0089 |
| 122 | 3BrC6 | 1.4008 | 1.03 | 0.7533 | -7.0199 | 1.1799 | 1.1556 | 0.0243 |
| 123 | 2m1BrC5 | 1.2741 | 1.03 | 0.8540 | -6.9967 | 1.1624 | 1.1664 | -0.0040 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 124 | 3m1BrC5 | 1.2495 | 1.03 | 0.8753 | -6.9896 | 1.1829 | 1.1690 | 0.0139 |
| 125 | 4m1BrC5 | 1.2398 | 1.03 | 0.8540 | -6.9886 | 1.1683 | 1.1679 | 0.0004 |
| 126 | 3m3BrC5 | 1.5178 | 1.03 | 0.8753 | -7.0476 | 1.1835 | 1.1581 | 0.0254 |
| 127 | 33mm1BrC4 | 1.2592 | 1.03 | 1.0264 | -7.0130 | 1.1556 | 1.1751 | -0.0195 |
| 128 | C7Br | 1.2414 | 1.03 | 0.9866 | -7.9861 | 1.1400 | 1.1320 | 0.0080 |
| 129 | 2BrC7 | 1.3755 | 1.03 | 0.9866 | -8.0165 | 1.1277 | 1.1271 | 0.0006 |
| 130 | 4BrC7 | 1.4243 | 1.03 | 0.9866 | -8.0269 | 1.1351 | 1.1254 | 0.0097 |
| 131 | C9Br | 1.2498 | 1.03 | 1.4718 | -9.9849 | 1.0840 | 1.0884 | -0.0044 |
| 132 | C10Br | 1.2527 | 1.03 | 1.7204 | -10.9812 | 1.0702 | 1.0722 | -0.0020 |
| 133 | PrCl | 1.1887 | 0.78 | 0.1356 | -3.9385 | 0.8899 | 0.9195 | -0.0296 |
| 134 | i-PrCl | 1.2810 | 0.78 | 0.1356 | -3.9604 | 0.8617 | 0.9153 | -0.0536 |
| 135 | n-BuCl | 1.2122 | 0.78 | 0.3203 | -4.9612 | 0.8862 | 0.9046 | -0.0184 |
| 136 | s-BuCl | 1.3292 | 0.78 | 0.3203 | -4.9881 | 0.8732 | 0.9004 | -0.0272 |
| 137 | i-BuCl | 1.2368 | 0.78 | 0.3921 | -4.9753 | 0.8773 | 0.9073 | -0.0300 |
| 138 | t-BuCl | 1.4215 | 0.78 | 0.3921 | -5.0166 | 0.8420 | 0.9007 | -0.0587 |
| 139 | C5Cl | 1.2260 | 0.78 | 0.5296 | -5.9741 | 0.8820 | 0.8967 | -0.0147 |
| 140 | 2ClC5 | 1.3527 | 0.78 | 0.5296 | -6.0031 | 0.8698 | 0.8928 | -0.0230 |
| 141 | 3ClC5 | 1.3773 | 0.78 | 0.5296 | -6.0085 | 0.8731 | 0.8920 | -0.0189 |
| 142 | 3m1ClC4 | 1.2357 | 0.78 | 0.6219 | -5.9831 | 0.8750 | 0.9008 | -0.0258 |
| 143 | 2m2ClC4 | 1.4697 | 0.78 | 0.6219 | -6.0346 | 0.8653 | 0.8938 | -0.0285 |
| 144 | 22mm1ClC3 | 1.2849 | 0.78 | 0.7552 | -6.0071 | 0.8660 | 0.9053 | -0.0393 |
| 145 | C6Cl | 1.2350 | 0.78 | 0.7533 | -6.9826 | 0.8785 | 0.8919 | -0.0134 |
| 146 | 3ClC6 | 1.4008 | 0.78 | 0.7533 | -7.0199 | 0.8684 | 0.8875 | -0.0191 |
| 147 | 2m2ClC5 | 1.4932 | 0.78 | 0.8540 | -7.0439 | 0.8630 | 0.8897 | -0.0267 |
| 148 | 4m2ClC5 | 1.3762 | 0.78 | 0.8540 | -7.0195 | 0.8610 | 0.8926 | -0.0316 |
| 149 | 2eClC4 | 1.2838 | 0.78 | 0.8753 | -6.9976 | 0.8914 | 0.8963 | -0.0049 |
| 150 | 3m3ClC5 | 1.5178 | 0.78 | 0.8753 | -7.0476 | 0.8900 | 0.8903 | -0.0003 |
| 151 | 33mm1ClC4 | 1.2592 | 0.78 | 1.0264 | -7.0130 | 0.8670 | 0.9022 | -0.0352 |
| 152 | 23mm2ClC4 | 1.5178 | 0.78 | 0.9654 | -7.0532 | 0.8780 | 0.8942 | -0.0162 |
| 153 | 22mm3ClC4 | 1.4254 | 0.78 | 1.0264 | -7.0553 | 0.8767 | 0.8971 | -0.0204 |
| 154 | C7Cl | 1.2414 | 0.78 | 0.9866 | -7.9861 | 0.8758 | 0.8891 | -0.0133 |
| 155 | 2ClC7 | 1.3755 | 0.78 | 0.9866 | -8.0165 | 0.8672 | 0.8859 | -0.0187 |
| 156 | 3ClC7 | 1.4146 | 0.78 | 0.9866 | -8.0249 | 0.8960 | 0.8850 | 0.0110 |
| 157 | 4ClC7 | 1.4243 | 0.78 | 0.9866 | -8.0269 | 0.8710 | 0.8848 | -0.0138 |
| 158 | 3m1ClC6 | 1.2585 | 0.78 | 1.1214 | -7.9911 | 0.8766 | 0.8947 | -0.0181 |
| 159 | 2m2ClC6 | 1.5070 | 0.78 | 1.0914 | -8.0483 | 0.8635 | 0.8872 | -0.0237 |
| 160 | 5m2ClC6 | 1.3803 | 0.78 | 1.0914 | -8.0220 | 0.8630 | 0.8900 | -0.0270 |
| 161 | 3m3ClC6 | 1.5413 | 0.78 | 1.1214 | -8.0516 | 0.8787 | 0.8882 | -0.0095 |
| 162 | 24mm2ClC5 | 1.5167 | 0.78 | 1.1998 | -8.0519 | 0.8610 | 0.8917 | -0.0307 |
| 163 | 22mm4ClC5 | 1.3997 | 0.78 | 1.2794 | -8.0308 | 0.8550 | 0.8976 | -0.0426 |
| 164 | 3e3ClC5 | 1.5659 | 0.78 | 1.1517 | -8.0529 | 0.8856 | 0.8895 | -0.0039 |
| 165 | C8Cl | 1.2461 | 0.78 | 1.2266 | -8.9872 | 0.8738 | 0.8873 | -0.0135 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 166 | 3m3ClC7 | 1.5551 | 0.78 | 1.3679 | -9.0522 | 0.8764 | 0.8869 | -0.0105 |
| 167 | 4m4ClC7 | 1.5648 | 0.78 | 1.3765 | -9.0519 | 0.8690 | 0.8872 | -0.0182 |
| 168 | 23mm3ClC6 | 1.5894 | 0.78 | 1.4990 | -9.0581 | 0.8869 | 0.8916 | -0.0047 |
| 169 | 2eClC6 | 1.3066 | 0.78 | 1.3679 | -9.0002 | 0.8769 | 0.8919 | -0.0150 |
| 170 | 244mmm2ClC5 | 1.5402 | 0.78 | 1.6445 | -9.0566 | 0.8746 | 0.8978 | -0.0232 |
| 171 | C9Cl | 1.2498 | 0.78 | 1.4718 | -9.9849 | 0.8720 | 0.8864 | -0.0144 |
| 172 | 2ClC9 | 1.3866 | 0.78 | 1.4718 | -10.0157 | 0.8790 | 0.8837 | -0.0047 |
| 173 | 4m4ClC8 | 1.5786 | 0.78 | 1.6299 | -10.0496 | 0.8723 | 0.8866 | -0.0143 |
| 174 | 3e3ClC7 | 1.6032 | 0.78 | 1.6668 | -10.0496 | 0.8856 | 0.8880 | -0.0024 |
| 175 | 223mmm3ClC6 | 1.6375 | 0.78 | 1.9732 | -10.0589 | 0.9010 | 0.8987 | 0.0023 |
| 176 | C10Cl | 1.2527 | 0.78 | 1.7204 | -10.9812 | 0.8705 | 0.8858 | -0.0153 |
| 177 | MeI | 1.0000 | 1.39 | 0.0000 | -1.8540 | 2.2790 | 2.2042 | 0.0748 |
| 178 | EtI | 1.1405 | 1.39 | 0.0000 | -2.9045 | 1.9358 | 1.8661 | 0.0697 |
| 179 | PrI | 1.1887 | 1.39 | 0.1356 | -3.9385 | 1.7489 | 1.6800 | 0.0689 |
| 180 | i-PrI | 1.2810 | 1.39 | 0.1356 | -3.9604 | 1.7042 | 1.6696 | 0.0346 |
| 181 | iBuI | 1.2368 | 1.39 | 0.3921 | -4.9753 | 1.6035 | 1.5606 | 0.0429 |
| 182 | C5I | 1.2260 | 1.39 | 0.5296 | -5.9741 | 1.5161 | 1.4699 | 0.0462 |
| 183 | 2IC5 | 1.3527 | 1.39 | 0.5296 | -6.0031 | 1.5096 | 1.4607 | 0.0489 |
| 184 | 3IC5 | 1.3773 | 1.39 | 0.5296 | -6.0085 | 1.5176 | 1.4590 | 0.0586 |
| 185 | 22mmC3I | 1.2849 | 1.39 | 0.7552 | -6.0071 | 1.4940 | 1.4808 | 0.0132 |
| 186 | C6I | 1.2350 | 1.39 | 0.7533 | -6.9826 | 1.4397 | 1.4034 | 0.0363 |
| 187 | C7I | 1.2414 | 1.39 | 0.9866 | -7.9861 | 1.3791 | 1.3512 | 0.0279 |
| 188 | 2IC7 | 1.3755 | 1.39 | 0.9866 | -8.0165 | 1.3040 | 1.3441 | -0.0401 |
| 189 | C8I | 1.2461 | 1.39 | 1.2266 | -8.9872 | 1.3297 | 1.3090 | 0.0207 |
| 190 | 2IC8 | 1.3819 | 1.39 | 1.2266 | -9.0179 | 1.3251 | 1.3026 | 0.0225 |
| 191 | PrSH | 1.1887 | 0.87 | 0.1356 | -3.9385 | 0.8411 | 0.8330 | 0.0081 |
| 192 | iPrSH | 1.2810 | 0.87 | 0.1356 | -3.9604 | 0.8143 | 0.8269 | -0.0126 |
| 193 | BuSH | 1.2122 | 0.87 | 0.3203 | -4.9612 | 0.8416 | 0.8318 | 0.0098 |
| 194 | s-BuSH | 1.3292 | 0.87 | 0.3203 | -4.9881 | 0.8295 | 0.8255 | 0.0040 |
| 195 | i-BuSH | 1.2368 | 0.87 | 0.3921 | -4.9753 | 0.8357 | 0.8335 | 0.0022 |
| 196 | t-BuSH | 1.4215 | 0.87 | 0.3921 | -5.0166 | 0.7943 | 0.8237 | -0.0294 |
| 197 | C5SH | 1.2260 | 0.87 | 0.5296 | -5.9741 | 0.8500 | 0.8336 | 0.0164 |
| 198 | 2SHC5 | 1.3527 | 0.87 | 0.5296 | -6.0031 | 0.8327 | 0.8276 | 0.0051 |
| 199 | 3SHC5 | 1.3773 | 0.87 | 0.5296 | -6.0085 | 0.8410 | 0.8265 | 0.0145 |
| 200 | 2mC4SH | 1.2603 | 0.87 | 0.6219 | -5.9889 | 0.8420 | 0.8358 | 0.0062 |
| 201 | 3mC4SH | 1.2357 | 0.87 | 0.6219 | -5.9831 | 0.8350 | 0.8370 | -0.0020 |
| 202 | 2m2SHC4 | 1.4697 | 0.87 | 0.6219 | -6.0346 | 0.8120 | 0.8262 | -0.0142 |
| 203 | C6SH | 1.2350 | 0.87 | 0.7533 | -6.9826 | 0.8424 | 0.8361 | 0.0063 |
| 204 | 2SHC6 | 1.3665 | 0.87 | 0.7533 | -7.0125 | 0.8345 | 0.8306 | 0.0039 |
| 205 | C7SH | 1.2414 | 0.87 | 0.9866 | -7.9861 | 0.8427 | 0.8390 | 0.0037 |
| 206 | C8SH | 1.2461 | 0.87 | 1.2266 | -8.9872 | 0.8433 | 0.8419 | 0.0014 |
| 207 | 2SHC8 | 1.3819 | 0.87 | 1.2266 | -9.0179 | 0.8366 | 0.8373 | -0.0007 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 208 | C10SH | 1.2527 | 0.87 | 1.7204 | -10.9812 | 0.8443 | 0.8474 | -0.0031 |
| 209 | C5F | 1.2260 | 0.41 | 0.5296 | -5.9741 | 0.7907 | 0.8439 | -0.0532 |
| 210 | C6F | 1.2350 | 0.41 | 0.7533 | -6.9826 | 0.7995 | 0.8459 | -0.0464 |
| 211 | 2FC6 | 1.3665 | 0.41 | 0.7533 | -7.0125 | 0.7916 | 0.8461 | -0.0545 |
| 212 | C7F | 1.2414 | 0.41 | 0.9866 | -7.9861 | 0.8062 | 0.8484 | -0.0422 |
| 213 | C8F | 1.2461 | 0.41 | 1.2266 | -8.9872 | 0.8108 | 0.8508 | -0.0400 |

[a] m, methyl; e, ethyl; for example 2mmC3 represent 2,2-dimethyl-propane. [b] from ref. 8. [c] Calculated by eq 8. [d] $\Delta = D_{exp.} - D_{calc.}$

**Table 7** Predictive Ability of equation 9

| no | RX [a] | $D_{exp.}$ ($g \cdot cm^{-3}$) | $D_{pred.}$ [b] ($g \cdot cm^{-3}$) | $D_{pred.}$ [c] ($g \cdot cm^{-3}$) | no | RX [a] | $D_{exp.}$ ($g \cdot cm^{-3}$) | $D_{pred.}$ [b] ($g \cdot cm^{-3}$) | $D_{pred.}$ [c] ($g \cdot cm^{-3}$) |
|---|---|---|---|---|---|---|---|---|---|
| 2 | i-PrNH2 | 0.6891 | 0.7147 | 0.7171 | 105 | 26mm4OHC8 | 0.8114 | 0.8311 | 0.8308 |
| 6 | C5NH2 | 0.7544 | 0.7535 | 0.7548 | 117 | 2m1BrC4 | 1.2234 | 1.2066 | 1.2062 |
| 15 | 4NC7 | 0.7670 | 0.7718 | 0.7737 | 123 | 2m1BrC5 | 1.1624 | 1.1669 | 1.1664 |
| 17 | 4m2NC6 | 0.7655 | 0.7785 | 0.7799 | 125 | 4m1BrC5 | 1.1683 | 1.1687 | 1.1679 |
| 25 | n-BuOH | 0.8098 | 0.7818 | 0.7818 | 126 | 3m3BrC5 | 1.1835 | 1.1564 | 1.1581 |
| 26 | s-BuOH | 0.8063 | 0.7783 | 0.7792 | 128 | C7Br | 1.1400 | 1.1325 | 1.1320 |
| 30 | 2OHC5 | 0.8094 | 0.7884 | 0.7893 | 132 | C10Br | 1.0702 | 1.0731 | 1.0722 |
| 34 | 2m2OHC4 | 0.8096 | 0.7902 | 0.7915 | 139 | C5Cl | 0.8820 | 0.8968 | 0.8967 |
| 41 | 3m2OHC5 | 0.8307 | 0.8025 | 0.8029 | 151 | 33mm1ClC4 | 0.8670 | 0.9033 | 0.9022 |
| 49 | OHC7 | 0.8219 | 0.8078 | 0.8076 | 152 | 23mm2ClC4 | 0.8780 | 0.8932 | 0.8942 |
| 58 | 2m3OHC6 | 0.8407 | 0.8081 | 0.8086 | 158 | 3m1ClC6 | 0.8766 | 0.8953 | 0.8947 |
| 63 | 22mm3OHC5 | 0.8253 | 0.8161 | 0.8161 | 172 | 2ClC9 | 0.8790 | 0.8835 | 0.8837 |
| 65 | 2OHC8 | 0.8193 | 0.8118 | 0.8121 | 177 | MeI | 2.2790 | 2.2210 | 2.2042 |
| 69 | 2m3OHC7 | 0.8235 | 0.8147 | 0.8151 | 180 | i-PrI | 1.7042 | 1.6691 | 1.6696 |
| 70 | 4m4OHC7 | 0.8248 | 0.8155 | 0.8162 | 191 | PrSH | 0.8411 | 0.8306 | 0.8330 |
| 73 | 25mm2OHC6 | 0.8227 | 0.8181 | 0.8184 | 200 | 2mC4SH | 0.8420 | 0.8339 | 0.8358 |
| 86 | 2OHC9 | 0.8471 | 0.8179 | 0.8180 | 202 | 2m2SHC4 | 0.8120 | 0.8225 | 0.8262 |
| 89 | 5OHC9 | 0.8356 | 0.8169 | 0.8172 | 205 | C7SH | 0.8427 | 0.8376 | 0.8390 |
| 90 | 2m2OHC8 | 0.8210 | 0.8197 | 0.8201 | 210 | C6F | 0.7995 | 0.8483 | 0.8459 |
| 102 | 2OHC10 | 0.8250 | 0.8231 | 0.8230 | 211 | 2FC6 | 0.7916 | 0.8478 | 0.8461 |

[a] m, methyl; e, ethyl; for example 2mmC3 represent 2,2-dimethyl-propane. [b] Predicated by eq 9. [c] Calculated by eq 8

## Conclusion

The above results imply that molecular volume can be calculated by perturbation theory for monosubstituted alkanes well. This method (eq 5 and eq 8) is reliable for estimating the density of alkanes RH and monosubstituted alkanes RX. Therefore eqs 5 and 8 were suggested to calculate the density for the alkanes and monosubstituted alkanes whose density is not determined experimentally yet. The Table 8 and 9 list the predicted density of 160 alkanes (including 150 alkanes with 1-10 carbon atoms and 10 normal chain alkanes with 11-20 carbon atoms) and some monosubstituted alkanes RX by eqs 5 and 8 respectively, which provide reference densities data for chemical engineering and petrochemical industries.

**Table 8** The Predicted Density(25°C) by eq 5 for 160 alkanes

| no. | Alkane | $D_{calc.}$[a] □g·cm$^{-3}$□ | no. | Alkane | $D_{calc.}$[a] □g·cm$^{-3}$□ |
|---|---|---|---|---|---|
| 1 | methane | 0.3156 | 81 | 2,2-dimethyloctane | 0.7339 |
| 2 | ethane | 0.4318 | 82 | 2,3-dimethyloctane | 0.7334 |
| 3 | propane | 0.5073 | 83 | 2,4-dimethyloctane | 0.7325 |
| 4 | butane | 0.5615 | 84 | 2,5-dimethyloctane | 0.7328 |
| 5 | 2-methylpropane | 0.5656 | 85 | 2,6-dimethyloctane | 0.7316 |
| 6 | pentane | 0.6030 | 86 | 2,7-dimethyloctane | 0.7295 |
| 7 | 2-methylbutane | 0.6082 | 87 | 3,3-dimethyloctane | 0.7379 |
| 8 | 2,2-dimehtylpropane | 0.6156 | 88 | 3,4-dimethyloctane | 0.7363 |
| 9 | hexane | 0.6357 | 89 | 3,5-dimethyloctane | 0.7353 |
| 10 | 2-methylpentane | 0.6412 | 90 | 3,6-dimethyloctane | 0.7340 |
| 11 | 3-methylpentane | 0.6426 | 91 | 4,4-dimethyloctane | 0.7396 |
| 12 | 2,2-dimehtylbutane | 0.6493 | 92 | 4,5-dimethyloctane | 0.7371 |
| 13 | 2,3-dimethylbutane | 0.6475 | 93 | 3-ethyloctane | 0.7297 |
| 14 | heptane | 0.6625 | 94 | 4-ethyloctane | 0.7310 |
| 15 | 2-methylhexane | 0.6678 | 95 | 2,2,3-trimethylheptane | 0.7435 |
| 16 | 3-methylhexane | 0.6698 | 96 | 2,2,4-trimethylheptane | 0.7431 |
| 17 | 2,2-dimethylpentane | 0.6780 | 97 | 2,2,5-trimethylheptane | 0.7416 |
| 18 | 2,3-dimethylpentane | 0.6763 | 98 | 2,2,6-trimethylheptane | 0.7391 |
| 19 | 2,4-dimethylpentane | 0.6737 | 99 | 2,3,3-trimethylheptane | 0.7420 |
| 20 | 3,3-dimethylpentane | 0.6806 | 100 | 2,3,4-trimethylheptane | 0.7435 |
| 21 | 3-ethylpentane | 0.6717 | 101 | 2,3,5-trimethylheptane | 0.7414 |
| 22 | 2,2,3-trimethylbutane | 0.6852 | 102 | 2,3,6-trimethylheptane | 0.7387 |
| 23 | octane | 0.6846 | 103 | 2,4,4-trimethylheptane | 0.7455 |
| 24 | 2-methylheptane | 0.6899 | 104 | 2,4,5-trimethylheptane | 0.7419 |
| 25 | 3-methylheptane | 0.6920 | 105 | 2,4,6-trimethylheptane | 0.7387 |
| 26 | 4-methylheptane | 0.6926 | 106 | 2,5,5-trimethylheptane | 0.7434 |
| 27 | 2,2-dimethylhexane | 0.7000 | 107 | 3,3,4-trimethylheptane | 0.7446 |
| 28 | 2,3-dimethylhexane | 0.6989 | 108 | 3,3,5-trimethylheptane | 0.7463 |
| 29 | 2,4-dimethylhexane | 0.6977 | 109 | 3,4,4-trimethylheptane | 0.7495 |
| 30 | 2,5-dimethylhexane | 0.6953 | 110 | 3,4,5-trimethylheptane | 0.7454 |
| 31 | 3,3-dimethylhexane | 0.7036 | 111 | 3-ethyl-2-methylheptane | 0.7373 |
| 32 | 3,4-dimethylhexane | 0.7008 | 112 | 4-ethyl-2-methylheptane | 0.7366 |
| 33 | 3-ethylhexane | 0.6947 | 113 | 5-ethyl-2-methylheptane | 0.7349 |
| 34 | 2,2,3-trimethylpentane | 0.7087 | 114 | 3-ethyl-3-methylheptane | 0.7427 |
| 35 | 2,2,4-trimethylpentane | 0.7061 | 115 | 4-ethyl-3-methylheptane | 0.7400 |
| 36 | 2,3,3-trimethylpentane | 0.7110 | 116 | 5-ethyl-3-methylheptane | 0.7321 |
| 37 | 2,3,4-trimethylpentane | 0.7056 | 117 | 3-ethyl-4-methylheptane | 0.7397 |
| 38 | 3-ethyl-2-methylpentane | 0.7013 | 118 | 4-ethyl-4-methylheptane | 0.7441 |
| 39 | 3-ethyl-3-methylpentane | 0.7066 | 119 | 4-propylheptane | 0.7320 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 2,2,3,3-tetramethylbutane | 0.7196 | 120 | 4-isopropylheptane | 0.7244 |
| 41 | nonane | 0.7035 | 121 | 2,2,3,3-tetrahexane | 0.7590 |
| 42 | 2-methyloctane | 0.7085 | 122 | 2,2,3,4-tetrahexane | 0.7543 |
| 43 | 3-methyloctane | 0.7107 | 123 | 2,2,3,5-tetrahexane | 0.7505 |
| 44 | 4-methyloctane | 0.7109 | 124 | 2,2,4,4-tetrahexane | 0.7547 |
| 45 | 2,2-dimethylheptane | 0.7183 | 125 | 2,2,4,5-tetrahexane | 0.7494 |
| 46 | 2,3-dimethylheptane | 0.7165 | 126 | 2,2,5,5-tetrahexane | 0.7494 |
| 47 | 2,4-dimethylheptane | 0.7171 | 127 | 2,3,3,4-tetrahexane | 0.7563 |
| 48 | 2,5-dimethylheptane | 0.7214 | 128 | 2,3,3,5-tetrahexane | 0.7526 |
| 49 | 2,6-dimethylheptane | 0.7199 | 129 | 2,3,4,4-tetrahexane | 0.7559 |
| 50 | 3,3-dimethylheptane | 0.7223 | 130 | 2,3,4,5-tetrahexane | 0.7502 |
| 51 | 3,4-dimethylheptane | 0.7202 | 131 | 3,3,4,4-tetrahexane | 0.7623 |
| 52 | 3,5-dimethylheptane | 0.7185 | 132 | 2,2-dimethyl-3-ethylhexane | 0.7447 |
| 53 | 4,4-dimethylheptane | 0.7234 | 133 | 2,2-dimethyl-4-ethylhexane | 0.7482 |
| 54 | 3-ethylheptane | 0.7137 | 134 | 2,3-dimethyl-3-ethylhexane | 0.7514 |
| 55 | 4-ethylheptane | 0.7146 | 135 | 2,3-dimethyl-4-ethylhexane | 0.7462 |
| 56 | 2,2,3-trimethylhexane | 0.7289 | 136 | 2,4-dimethyl-3-ethylhexane | 0.7467 |
| 57 | 2,2,4-trimethylhexane | 0.7267 | 137 | 2,4-dimethyl-4-ethylhexane | 0.7487 |
| 58 | 2,2,5-trimethylhexane | 0.7239 | 138 | 2,5-dimethyl-3-ethylhexane | 0.7430 |
| 59 | 2,3,3-trimethylhexane | 0.7306 | 139 | 3,3-dimethyl-4-ethylhexane | 0.7520 |
| 60 | 2,3,4-trimethylhexane | 0.7268 | 140 | 3,4-dimethyl-3-ethylhexane | 0.7530 |
| 61 | 2,3,5-trimethylhexane | 0.7234 | 141 | 3,3-diethylhexane | 0.7476 |
| 62 | 2,4,4-trimethylhexane | 0.7283 | 142 | 3,4-diethylhexane | 0.7510 |
| 63 | 3,3,4-trimethylhexane | 0.7323 | 143 | 3-isopropyl-2-methylhexane | 0.7451 |
| 64 | 3-ethyl-2-methylhexane | 0.7210 | 144 | 2,2,3,3,4-pentamethylpentane | 0.7825 |
| 65 | 4-ethyl-2-methylhexane | 0.7186 | 145 | 2,2,3,4,4-pentamethylpentane | 0.7636 |
| 66 | 3-ethyl-3-methylhexane | 0.7266 | 146 | 3-ethyl-2,2,3-trimethylpentane | 0.7629 |
| 67 | 4-ethyl-2-methylhexane | 0.7228 | 147 | 3-ethyl-2,2,4-trimethylpentane | 0.7559 |
| 68 | 2,2,3,3-tetramethylpentane | 0.7421 | 148 | 3-ethyl-2,3,4-trimethylpentane | 0.7591 |
| 69 | 2,2,3,4-tetramethylpentane | 0.7334 | 149 | 3,3-diethyl-2-methylpentane | 0.7553 |
| 70 | 2,2,4,4-tetramethylpentane | 0.7353 | 150 | 2,4-dimethyl-3-isopropylpentane | 0.7523 |
| 71 | 2,3,3,4-tetramethylpentane | 0.7382 | 151 | undecane | 0.7337 |
| 72 | 2,2-dimethyl-3-ethylpentane | 0.7318 | 152 | dodecane | 0.7461 |
| 73 | 2,3-dimethyl-3-ethylpentane | 0.7331 | 153 | tridecane | 0.7570 |
| 74 | 2,4-dimethyl-3-ethylpentane | 0.7265 | 154 | tetradecane | 0.7668 |
| 75 | 3,3-diethylpentane | 0.7300 | 155 | pentadecane | 0.7756 |
| 76 | decane | 0.7197 | 156 | hexadecane | 0.7835 |
| 77 | 2-methylnonane | 0.7245 | 157 | heptadecane | 0.7908 |
| 78 | 3-methylnonane | 0.7266 | 158 | octadecane | 0.7973 |
| 79 | 4-methylnonane | 0.7276 | 159 | nonadecane | 0.8034 |
| 80 | 5-methylnonane | 0.7279 | 160 | eicosane | 0.8090 |

[a] Calculated by eq 5

**Table 9** The Predicted Density(20°C) by eq 8 for some monosubstituted alkanes RX

| no | RX [a] | $D_{calc.}$ [b] (g·cm$^{-3}$) | no | RX [a] | $D_{calc.}$ [b] (g·cm$^{-3}$) | no | RX [a] | $D_{calc.}$ [b] (g·cm$^{-3}$) |
|---|---|---|---|---|---|---|---|---|
| 1 | MeOH | 0.7660 | 202 | MeSH | 0.8824 | 403 | MeNH2 | 0.6825 |
| 2 | EtOH | 0.7618 | 203 | EtSH | 0.8421 | 404 | EtNH2 | 0.6996 |
| 3 | PrOH | 0.7713 | 204 | PrSH | 0.8330 | 405 | PrNH2 | 0.7211 |
| 4 | iPrOH | 0.7170 | 205 | iPrSH | 0.8269 | 406 | iPrNH2 | 0.6918 |
| 5 | n-BuOH | 0.7818 | 206 | n-BuSH | 0.8318 | 407 | n-BuNH2 | 0.7394 |
| 6 | s-BuOH | 0.7792 | 207 | s-BuSH | 0.8255 | 408 | s-BuNH2 | 0.7352 |
| 7 | i-BuOH | 0.7846 | 208 | i-BuSH | 0.8335 | 409 | i-BuNH2 | 0.7415 |
| 8 | t-BuOH | 0.7806 | 209 | t-BuSH | 0.8237 | 410 | t-BuNH2 | 0.7351 |
| 9 | C5OH | 0.7917 | 210 | C5SH | 0.8336 | 411 | C5NH2 | 0.7548 |
| 10 | 2OHC5 | 0.7893 | 211 | 2SHC5 | 0.8276 | 412 | 2NC5 | 0.7509 |
| 11 | 3OHC5 | 0.7888 | 212 | 3SHC5 | 0.8265 | 413 | 3NC5 | 0.7501 |
| 12 | 22mm1OHC3 | 0.8005 | 213 | 22mm1SHC3 | 0.8401 | 414 | 22mm1NC3 | 0.7621 |
| 13 | 3mOHC4 | 0.7957 | 214 | 3mSHC4 | 0.8370 | 415 | 3mNC4 | 0.7584 |
| 14 | 2m2OHC4 | 0.7914 | 215 | 2m2SHC4 | 0.8262 | 416 | 2m2NC4 | 0.7513 |
| 15 | 3m2OHC4 | 0.7930 | 216 | 3m2SHC4 | 0.8304 | 417 | 3m2NC4 | 0.7540 |
| 16 | OHC6 | 0.8001 | 217 | SHC6 | 0.8361 | 418 | C6NH2 | 0.7674 |
| 17 | 2OHC6 | 0.7979 | 218 | 2SHC6 | 0.8306 | 419 | 2NC6 | 0.7638 |
| 18 | 2mOHC5 | 0.8038 | 219 | 2mSHC5 | 0.8385 | 420 | 2m1NC5 | 0.7703 |
| 19 | 3mOHC5 | 0.8054 | 220 | 3mSHC5 | 0.8407 | 421 | 3m1NC5 | 0.7722 |
| 20 | 4mOHC5 | 0.8044 | 221 | 4mSHC5 | 0.8400 | 422 | 4m1NC5 | 0.7713 |
| 21 | 3m2OHC5 | 0.8029 | 222 | 3m2SHC5 | 0.8344 | 423 | 3m2NC5 | 0.7680 |
| 22 | 4m2OHC5 | 0.8021 | 223 | 4m2SHC5 | 0.8343 | 424 | 4m2NC5 | 0.7676 |
| 23 | 2m3OHC5 | 0.8013 | 224 | 2m3SHC5 | 0.8323 | 425 | 2m3NC5 | 0.7663 |
| 24 | 3m3OHC5 | 0.8012 | 225 | 3m3SHC5 | 0.8298 | 426 | 3m3NC5 | 0.7651 |
| 25 | 22mmOHC4 | 0.8087 | 226 | 22mmSHC4 | 0.8423 | 427 | 22mm1NC4 | 0.7745 |
| 26 | 23mmOHC4 | 0.8089 | 227 | 23mmSHC4 | 0.8431 | 428 | 23mm1NC4 | 0.7750 |
| 27 | 23mm2OHC4 | 0.8049 | 228 | 23mm2SHC4 | 0.8333 | 429 | 23mm2NC4 | 0.7685 |
| 28 | 2eOHC4 | 0.8048 | 229 | 2eSHC4 | 0.8392 | 430 | 2e1NC4 | 0.7712 |
| 29 | OHC7 | 0.8076 | 230 | SHC7 | 0.8390 | 431 | C7NH2 | 0.7782 |
| 30 | 2OHC7 | 0.8056 | 231 | 2SHC7 | 0.8340 | 432 | 2NC7 | 0.7749 |
| 31 | 4OHC7 | 0.8049 | 232 | 4SHC7 | 0.8323 | 433 | 4NC7 | 0.7737 |
| 32 | 2mOHC6 | 0.8110 | 233 | 2mSHC6 | 0.8413 | 434 | 2m1NC6 | 0.7809 |
| 33 | 3mOHC6 | 0.8131 | 234 | 3mSHC6 | 0.8438 | 435 | 3m1NC6 | 0.7831 |
| 34 | 4mOHC6 | 0.8132 | 235 | 4mSHC6 | 0.8442 | 436 | 4m1NC6 | 0.7834 |
| 35 | 5mOHC6 | 0.8116 | 236 | 5mSHC6 | 0.8428 | 437 | 5m1NC6 | 0.7819 |
| 36 | 2m2OHC6 | 0.8079 | 237 | 2m2SHC6 | 0.8332 | 438 | 2m2NC6 | 0.7756 |
| 37 | 5m2OHC6 | 0.8096 | 238 | 5m2SHC6 | 0.8377 | 439 | 5m2NC6 | 0.7786 |
| 38 | 2m3OHC6 | 0.8086 | 239 | 2m3SHC6 | 0.8352 | 440 | 2m3NC6 | 0.7770 |
| 39 | 3m3OHC6 | 0.8091 | 240 | 3m3SHC6 | 0.8336 | 441 | 3m3NC6 | 0.7764 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 40 | 5m3OHC6 | 0.8090 | 241 | 5m3SHC6 | 0.8361 | 442 | 5m3NC6 | 0.7775 |
| 41 | 24mmOHC5 | 0.8155 | 242 | 24mmSHC5 | 0.8455 | 443 | 24mm1NC5 | 0.7851 |
| 42 | 24mm2OHC5 | 0.8123 | 243 | 24mm2SHC5 | 0.8371 | 444 | 24mm2NC5 | 0.7797 |
| 43 | 22mm3OHC5 | 0.8161 | 244 | 22mm3SHC5 | 0.8416 | 445 | 22mm3NC5 | 0.7836 |
| 44 | 24mm3OHC5 | 0.8129 | 245 | 24mm3SHC5 | 0.8386 | 446 | 24mm3NC5 | 0.7806 |
| 45 | 2OHC8 | 0.8121 | 246 | 2SHC8 | 0.8373 | 447 | 2NC8 | 0.7842 |
| 46 | 3OHC8 | 0.8116 | 247 | 3SHC8 | 0.8359 | 448 | 3NC8 | 0.7833 |
| 47 | 4OHC8 | 0.8114 | 248 | 4SHC8 | 0.8355 | 449 | 4NC8 | 0.7830 |
| 48 | 6m2OHC7 | 0.8160 | 249 | 6m2SHC7 | 0.8409 | 450 | 6m2NC7 | 0.7878 |
| 49 | 2m3OHC7 | 0.8151 | 250 | 2m3SHC7 | 0.8384 | 451 | 2m3NC7 | 0.7861 |
| 50 | 4m4OHC7 | 0.8162 | 251 | 4m4SHC7 | 0.8373 | 452 | 4m4NC7 | 0.7862 |
| 51 | 25mmOHC6 | 0.8213 | 252 | 25mmSHC6 | 0.8479 | 453 | 25mmNC6 | 0.7937 |
| 52 | 23mm2OHC6 | 0.8210 | 253 | 23mm2SHC6 | 0.8420 | 454 | 23mm2NC6 | 0.7908 |
| 53 | 25mm2OHC6 | 0.8184 | 254 | 25mm2SHC6 | 0.8403 | 455 | 25mm2NC6 | 0.7887 |
| 54 | 22mm3OHC6 | 0.8222 | 255 | 22mm3SHC6 | 0.8443 | 456 | 22mm3NC6 | 0.7925 |
| 55 | 25mm3OHC6 | 0.8190 | 256 | 25mm3SHC6 | 0.8418 | 457 | 25mm3NC6 | 0.7897 |
| 56 | 35mm3OHC6 | 0.8199 | 257 | 35mm3SHC6 | 0.8408 | 458 | 35mm3NC6 | 0.7897 |
| 57 | 44mm3OHC6 | 0.8252 | 258 | 44mm3SHC6 | 0.8471 | 459 | 44mm3NC6 | 0.7953 |
| 58 | 2eOHC6 | 0.8188 | 259 | 2eSHC6 | 0.8452 | 460 | 2eNC6 | 0.7912 |
| 59 | 3e3OHC6 | 0.8177 | 260 | 3e3SHC6 | 0.8382 | 461 | 3e3NC6 | 0.7874 |
| 60 | 244mmm2OHC5 | 0.8263 | 261 | 244mmm2SHC5 | 0.8472 | 462 | 244mmm2NC5 | 0.7959 |
| 61 | 224mmm3OHC5 | 0.8265 | 262 | 224mmm3SHC5 | 0.8478 | 463 | 224mmm3NC5 | 0.7963 |
| 62 | 234mmm3OHC5 | 0.8254 | 263 | 234mmm3SHC5 | 0.8448 | 464 | 234mmm3NC5 | 0.7943 |
| 63 | 3e2m2OHC5 | 0.8229 | 264 | 3e2m2SHC5 | 0.8436 | 465 | 3e2m2NC5 | 0.7925 |
| 64 | 3e2m3OHC5 | 0.8224 | 265 | 3e2m3SHC5 | 0.8420 | 466 | 3e2m3NC5 | 0.7915 |
| 65 | OHC9 | 0.8196 | 266 | SHC9 | 0.8448 | 467 | C9NH2 | 0.7951 |
| 66 | 2OHC9 | 0.8180 | 267 | 2SHC9 | 0.8405 | 468 | 2NC9 | 0.7923 |
| 67 | 3OHC9 | 0.8175 | 268 | 3SHC9 | 0.8392 | 469 | 3NC9 | 0.7915 |
| 68 | 4OHC9 | 0.8173 | 269 | 4SHC9 | 0.8387 | 470 | 4NC9 | 0.7911 |
| 69 | 5OHC9 | 0.8172 | 270 | 5SHC9 | 0.8385 | 471 | 5NC9 | 0.7910 |
| 70 | 2m2OHC8 | 0.8201 | 271 | 2m2SHC8 | 0.8399 | 472 | 2m2NC8 | 0.7931 |
| 71 | 4m4OHC8 | 0.8220 | 272 | 4m4SHC8 | 0.8406 | 473 | 4m4NC8 | 0.7944 |
| 72 | 26mm2OHC7 | 0.8284 | 273 | 26mm2SHC7 | 0.8477 | 474 | 26mm2NC7 | 0.8009 |
| 73 | 23mm3OHC7 | 0.8255 | 274 | 23mm3SHC7 | 0.8434 | 475 | 23mm3NC7 | 0.7975 |
| 74 | 26mm3OHC7 | 0.8290 | 275 | 26mm3SHC7 | 0.8491 | 476 | 26mm3NC7 | 0.8019 |
| 75 | 24mm4OHC7 | 0.8261 | 276 | 24mm4SHC7 | 0.8442 | 477 | 24mm4NC7 | 0.7981 |
| 76 | 26mm4OHC7 | 0.8290 | 277 | 26mm4SHC7 | 0.8493 | 478 | 26mm4NC7 | 0.8020 |
| 77 | 4e4OHC7 | 0.8242 | 278 | 4e4SHC7 | 0.8420 | 479 | 4e4NC7 | 0.7962 |
| 78 | 2e3mOHC6 | 0.8313 | 279 | 2e3mSHC6 | 0.8543 | 480 | 2e3m1NC6 | 0.8054 |
| 79 | 223mmm3OHC6 | 0.8342 | 280 | 223mmm3SHC6 | 0.8509 | 481 | 223mmm3NC6 | 0.8053 |
| 80 | 244mmm3OHC6 | 0.8347 | 281 | 244mmm3SHC6 | 0.8532 | 482 | 244mmm3NC6 | 0.8066 |
| 81 | OHC10 | 0.8246 | 282 | SHC10 | 0.8474 | 483 | C10NH2 | 0.8019 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 82 | 2OHC10 | 0.8230 | 283 | 2SHC10 | 0.8434 | 484 | 2NC10 | 0.7993 |
| 83 | 4OHC10 | 0.8224 | 284 | 4SHC10 | 0.8417 | 485 | 4NC10 | 0.7982 |
| 84 | 27mm3OHC8 | 0.8291 | 285 | 27mm3SHC8 | 0.8476 | 486 | 27mm3NC8 | 0.8043 |
| 85 | 26mm4OHC8 | 0.8308 | 286 | 26mm4SHC8 | 0.8491 | 487 | 26mm4NC8 | 0.8059 |
| 86 | 3e2m3OHC7 | 0.8339 | 287 | 3e2m3SHC7 | 0.8490 | 488 | 3e2m3NC7 | 0.8074 |
| 87 | MeF | 0.8968 | 288 | MeCl | 1.0277 | 489 | MeBr | 1.7066 |
| 88 | EtF | 0.8553 | 289 | EtCl | 0.9497 | 490 | EtBr | 1.4607 |
| 89 | PrF | 0.8448 | 290 | PrCl | 0.9195 | 491 | PrBr | 1.3349 |
| 90 | iPrF | 0.7499 | 291 | iPrCl | 0.8768 | 492 | iPrBr | 1.2931 |
| 91 | n-BuF | 0.8428 | 292 | n-BuCl | 0.9046 | 493 | n-BuBr | 1.2562 |
| 92 | s-BuF | 0.8429 | 293 | s-BuCl | 0.9004 | 494 | s-BuBr | 1.2493 |
| 93 | i-BuF | 0.8466 | 294 | i-BuCl | 0.9073 | 495 | i-BuBr | 1.2594 |
| 94 | t-BuF | 0.8470 | 295 | t-BuCl | 0.9007 | 496 | t-BuBr | 1.2486 |
| 95 | C5F | 0.8439 | 296 | C5Cl | 0.8967 | 497 | C5Br | 1.2022 |
| 96 | 2FC5 | 0.8441 | 297 | 2ClC5 | 0.8928 | 498 | 2BrC5 | 1.1960 |
| 97 | 3FC5 | 0.8441 | 298 | 3ClC5 | 0.8920 | 499 | 3BrC5 | 1.1949 |
| 98 | 22mm1FC3 | 0.8551 | 299 | 22mm1ClC3 | 0.9053 | 500 | 22mm1BrC3 | 1.2127 |
| 99 | 3mFC4 | 0.8486 | 300 | 3m1ClC4 | 0.9008 | 501 | 3mBrC4 | 1.2074 |
| 100 | 2m2FC4 | 0.8492 | 301 | 2m2ClC4 | 0.8938 | 502 | 2m2BrC4 | 1.1962 |
| 101 | 3m2FC4 | 0.8488 | 302 | 3m2ClC4 | 0.8964 | 503 | 3m2BrC4 | 1.2005 |
| 102 | C6F | 0.8459 | 303 | ClC6 | 0.8919 | 504 | BrC6 | 1.1624 |
| 103 | 2FC6 | 0.8461 | 304 | 2ClC6 | 0.8884 | 505 | 2BrC6 | 1.1569 |
| 104 | 2mFC5 | 0.8507 | 305 | 2mClC5 | 0.8953 | 506 | 2mBrC5 | 1.1664 |
| 105 | 3mFC5 | 0.8520 | 306 | 3mClC5 | 0.8973 | 507 | 3mBrC5 | 1.1690 |
| 106 | 4mFC5 | 0.8507 | 307 | 4mClC5 | 0.8963 | 508 | 4mBrC5 | 1.1679 |
| 107 | 3m2FC5 | 0.8522 | 308 | 3m2ClC5 | 0.8932 | 509 | 3m2BrC5 | 1.1627 |
| 108 | 4m2FC5 | 0.8509 | 309 | 4m2ClC5 | 0.8926 | 510 | 4m2BrC5 | 1.1621 |
| 109 | 2m3FC5 | 0.8510 | 310 | 2m3ClC5 | 0.8914 | 511 | 2m3BrC5 | 1.1602 |
| 110 | 3m3FC5 | 0.8527 | 311 | 3m3ClC5 | 0.8903 | 512 | 3m3BrC5 | 1.1581 |
| 111 | 22mmFC4 | 0.8568 | 312 | 22mmClC4 | 0.9002 | 513 | 22mmBrC4 | 1.1721 |
| 112 | 23mmFC4 | 0.8565 | 313 | 23mmClC4 | 0.9006 | 514 | 23mmBrC4 | 1.1728 |
| 113 | 23mm2FC4 | 0.8568 | 314 | 23mm2ClC4 | 0.8942 | 515 | 23mm2BrC4 | 1.1630 |
| 114 | 2eFC4 | 0.8520 | 315 | 2eClC4 | 0.8963 | 516 | 2eBrC4 | 1.1675 |
| 115 | FC7 | 0.8484 | 316 | ClC7 | 0.8891 | 517 | BrC7 | 1.1320 |
| 116 | 2FC7 | 0.8485 | 317 | 2ClC7 | 0.8859 | 518 | 2BrC7 | 1.1271 |
| 117 | 4FC7 | 0.8487 | 318 | 4ClC7 | 0.8848 | 519 | 4BrC7 | 1.1254 |
| 118 | 2mFC6 | 0.8528 | 319 | 2mClC6 | 0.8923 | 520 | 2mBrC6 | 1.1357 |
| 119 | 3mFC6 | 0.8546 | 320 | 3mClC6 | 0.8947 | 521 | 3mBrC6 | 1.1387 |
| 120 | 4mFC6 | 0.8546 | 321 | 4mClC6 | 0.8949 | 522 | 4mBrC6 | 1.1391 |
| 121 | 5mFC6 | 0.8528 | 322 | 5mClC6 | 0.8933 | 523 | 5mBrC6 | 1.1371 |
| 122 | 2m2FC6 | 0.8534 | 323 | 2m2ClC6 | 0.8872 | 524 | 2m2BrC6 | 1.1278 |
| 123 | 5m2FC6 | 0.8530 | 324 | 5m2ClC6 | 0.8900 | 525 | 5m2BrC6 | 1.1321 |

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|---|---|---|---|---|---|---|---|---|
| 124 | 2m3FC6 | 0.8532 | 325 | 2m3ClC6 | 0.8885 | 526 | 2m3BrC6 | 1.1298 |
| 125 | 3m3FC6 | 0.8554 | 326 | 3m3ClC6 | 0.8882 | 527 | 3m3BrC6 | 1.1288 |
| 126 | 5m3FC6 | 0.8531 | 327 | 5m3ClC6 | 0.8890 | 528 | 5m3BrC6 | 1.1306 |
| 127 | 24mmFC5 | 0.8578 | 328 | 24mmClC5 | 0.8970 | 529 | 24mmBrC5 | 1.1413 |
| 128 | 24mm2FC5 | 0.8584 | 329 | 24mm2ClC5 | 0.8917 | 530 | 24mm2BrC5 | 1.1332 |
| 129 | 22mm3FC5 | 0.8618 | 330 | 22mm3ClC5 | 0.8960 | 531 | 22mm3BrC5 | 1.1387 |
| 130 | 24mm3FC5 | 0.8583 | 331 | 24mm3ClC5 | 0.8927 | 532 | 24mm3BrC5 | 1.1347 |
| 131 | 2FC8 | 0.8509 | 332 | 2ClC8 | 0.8844 | 533 | 2BrC8 | 1.1035 |
| 132 | 3FC8 | 0.8511 | 333 | 3ClC8 | 0.8836 | 534 | 3BrC8 | 1.1022 |
| 133 | 4FC8 | 0.8511 | 334 | 4ClC8 | 0.8833 | 535 | 4BrC8 | 1.1018 |
| 134 | 6m2FC7 | 0.8552 | 335 | 6m2ClC7 | 0.8884 | 536 | 6m2BrC7 | 1.1083 |
| 135 | 2m3FC7 | 0.8554 | 336 | 2m3ClC7 | 0.8868 | 537 | 2m3BrC7 | 1.1059 |
| 136 | 4m4FC7 | 0.8583 | 337 | 4m4ClC7 | 0.8872 | 538 | 4m4BrC7 | 1.1057 |
| 137 | 25mmFC6 | 0.8594 | 338 | 25mmClC6 | 0.8946 | 539 | 25mmBrC6 | 1.1163 |
| 138 | 23mm2FC6 | 0.8634 | 339 | 23mm2ClC6 | 0.8923 | 540 | 23mm2BrC6 | 1.1118 |
| 139 | 25mm2FC6 | 0.8600 | 340 | 25mm2ClC6 | 0.8899 | 541 | 25mm2BrC6 | 1.1091 |
| 140 | 22mm3FC6 | 0.8637 | 341 | 22mm3ClC6 | 0.8939 | 542 | 22mm3BrC6 | 1.1142 |
| 141 | 25mm3FC6 | 0.8598 | 342 | 25mm3ClC6 | 0.8908 | 543 | 25mm3BrC6 | 1.1106 |
| 142 | 35mm3FC6 | 0.8623 | 343 | 35mm3ClC6 | 0.8911 | 544 | 35mm3BrC6 | 1.1103 |
| 143 | 44mm3FC6 | 0.8669 | 344 | 44mm3ClC6 | 0.8970 | 545 | 44mm3BrC6 | 1.1179 |
| 144 | 2eFC6 | 0.8569 | 345 | 2eClC6 | 0.8919 | 546 | 2eBrC6 | 1.1129 |
| 145 | 3e3FC6 | 0.8603 | 346 | 3e3ClC6 | 0.8886 | 547 | 3e3BrC6 | 1.1072 |
| 146 | 244mmm2FC5 | 0.8688 | 347 | 244mmm2ClC5 | 0.8978 | 548 | 244mmm2BrC5 | 1.1185 |
| 147 | 224mmm3FC5 | 0.8687 | 348 | 224mmm3ClC5 | 0.8982 | 549 | 224mmm3BrC5 | 1.1191 |
| 148 | 234mmm3FC5 | 0.8691 | 349 | 234mmm3ClC5 | 0.8964 | 550 | 234mmm3BrC5 | 1.1163 |
| 149 | 3e2m2FC5 | 0.8656 | 350 | 3e2m2ClC5 | 0.8942 | 551 | 3e2m2BrC5 | 1.1140 |
| 150 | 3e2m3FC5 | 0.8658 | 351 | 3e2m3ClC5 | 0.8933 | 552 | 3e2m3BrC5 | 1.1126 |
| 151 | FC9 | 0.8532 | 352 | ClC9 | 0.8864 | 553 | BrC9 | 1.0884 |
| 152 | 2FC9 | 0.8534 | 353 | 2ClC9 | 0.8837 | 554 | 2BrC9 | 1.0844 |
| 153 | 3FC9 | 0.8535 | 354 | 3ClC9 | 0.8829 | 555 | 3BrC9 | 1.0832 |
| 154 | 4FC9 | 0.8535 | 355 | 4ClC9 | 0.8826 | 556 | 4BrC9 | 1.0828 |
| 155 | 5FC9 | 0.8536 | 356 | 5ClC9 | 0.8825 | 557 | 5BrC9 | 1.0826 |
| 156 | 2m2FC8 | 0.8577 | 357 | 2m2ClC8 | 0.8850 | 558 | 2m2BrC8 | 1.0852 |
| 157 | 4m4FC8 | 0.8606 | 358 | 4m4ClC8 | 0.8866 | 559 | 4m4BrC8 | 1.0867 |
| 158 | 26mm2FC7 | 0.8667 | 359 | 26mm2ClC7 | 0.8935 | 560 | 26mm2BrC7 | 1.0953 |
| 159 | 23mm3FC7 | 0.8647 | 360 | 23mm3ClC7 | 0.8900 | 561 | 23mm3BrC7 | 1.0906 |
| 160 | 26mm3FC7 | 0.8665 | 361 | 26mm3ClC7 | 0.8944 | 562 | 26mm3BrC7 | 1.0966 |
| 161 | 24mm4FC7 | 0.8650 | 362 | 24mm4ClC7 | 0.8906 | 563 | 24mm4BrC7 | 1.0914 |
| 162 | 26mm4FC7 | 0.8665 | 363 | 26mm4ClC7 | 0.8945 | 564 | 26mm4BrC7 | 1.0967 |
| 163 | 4e4FC7 | 0.8634 | 364 | 4e4ClC7 | 0.8886 | 565 | 4e4BrC7 | 1.0889 |
| 164 | 2e3mFC6 | 0.8669 | 365 | 2e3mClC6 | 0.8978 | 566 | 2e3mBrC6 | 1.1015 |
| 165 | 223mmm3FC6 | 0.8746 | 366 | 223mmm3ClC6 | 0.8987 | 567 | 223mmm3BrC6 | 1.1007 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 166 | 244mmm3FC6 | 0.8737 | 367 | 244mmm3ClC6 | 0.8998 | 568 | 244mmm3BrC6 | 1.1026 |
| 167 | FC10 | 0.8555 | 368 | ClC10 | 0.8858 | 569 | BrC10 | 1.0722 |
| 168 | 2FC10 | 0.8556 | 369 | 2ClC10 | 0.8833 | 570 | 2BrC10 | 1.0686 |
| 169 | 4FC10 | 0.8558 | 370 | 4ClC10 | 0.8823 | 571 | 4BrC10 | 1.0670 |
| 170 | 27mm3FC8 | 0.8633 | 371 | 27mm3ClC8 | 0.8890 | 572 | 27mm3BrC8 | 1.0747 |
| 171 | 26mm4FC8 | 0.8652 | 372 | 26mm4ClC8 | 0.8907 | 573 | 26mm4BrC8 | 1.0767 |
| 172 | 3e2m3FC7 | 0.8707 | 373 | 3e2m3ClC7 | 0.8928 | 574 | 3e2m3BrC7 | 1.0782 |
| 173 | MeI | 2.2042 | 374 | 2IC7 | 1.3441 | 575 | 3e3IC6 | 1.3045 |
| 174 | EtI | 1.8661 | 375 | 4IC7 | 1.3416 | 576 | 244mmm2IC5 | 1.3177 |
| 175 | PrI | 1.6800 | 376 | 2mIC6 | 1.3548 | 577 | 224mmm3IC5 | 1.3185 |
| 176 | iPrI | 1.6611 | 377 | 3mIC6 | 1.3586 | 578 | 234mmm3IC5 | 1.3144 |
| 177 | n-BuI | 1.5575 | 378 | 4mIC6 | 1.3591 | 579 | 3e2m2IC5 | 1.3124 |
| 178 | s-BuI | 1.5472 | 379 | 5mIC6 | 1.3570 | 580 | 3e2m3IC5 | 1.3103 |
| 179 | i-BuI | 1.5606 | 380 | 2m2IC6 | 1.3433 | 581 | IC9 | 1.2743 |
| 180 | t-BuI | 1.5446 | 381 | 5m2IC6 | 1.3497 | 582 | 2IC9 | 1.2685 |
| 181 | C5I | 1.4699 | 382 | 2m3IC6 | 1.3461 | 583 | 3IC9 | 1.2667 |
| 182 | 2IC5 | 1.4607 | 383 | 3m3IC6 | 1.3439 | 584 | 4IC9 | 1.2661 |
| 183 | 3IC5 | 1.4590 | 384 | 5m3IC6 | 1.3474 | 585 | 5IC9 | 1.2659 |
| 184 | 22mm1IC3 | 1.4808 | 385 | 24mmIC5 | 1.3611 | 586 | 2m2IC8 | 1.2680 |
| 185 | 3mIC4 | 1.4756 | 386 | 24mm2IC5 | 1.3492 | 587 | 4m4IC8 | 1.2692 |
| 186 | 2m2IC4 | 1.4590 | 387 | 22mm3IC5 | 1.3559 | 588 | 26mm2IC7 | 1.2792 |
| 187 | 3m2IC4 | 1.4654 | 388 | 24mm3IC5 | 1.3514 | 589 | 23mm3IC7 | 1.2732 |
| 188 | IC6 | 1.4034 | 389 | 2IC8 | 1.3026 | 590 | 26mm3IC7 | 1.2811 |
| 189 | 2IC6 | 1.3953 | 390 | 3IC8 | 1.3007 | 591 | 24mm4IC7 | 1.2744 |
| 190 | 2mIC5 | 1.4073 | 391 | 4IC8 | 1.3001 | 592 | 26mm4IC7 | 1.2814 |
| 191 | 3mIC5 | 1.4106 | 392 | 6m2IC7 | 1.3080 | 593 | 4e4IC7 | 1.2713 |
| 192 | 4mIC5 | 1.4095 | 393 | 2m3IC7 | 1.3044 | 594 | 2e3mIC6 | 1.2881 |
| 193 | 3m2IC5 | 1.4013 | 394 | 4m4IC7 | 1.3031 | 595 | 223mmm3IC6 | 1.2841 |
| 194 | 4m2IC5 | 1.4011 | 395 | 25mmIC6 | 1.3179 | 596 | 244mmm3IC6 | 1.2871 |
| 195 | 2m3IC5 | 1.3981 | 396 | 23mm2IC6 | 1.3100 | 597 | IC10 | 1.2450 |
| 196 | 3m3IC5 | 1.3945 | 397 | 25mm2IC6 | 1.3074 | 598 | 2IC10 | 1.2397 |
| 197 | 22mmIC4 | 1.4133 | 398 | 22mm3IC6 | 1.3133 | 599 | 4IC10 | 1.2374 |
| 198 | 23mmIC4 | 1.4145 | 399 | 25mm3IC6 | 1.3096 | 600 | 27mm3IC8 | 1.2458 |
| 199 | 23mm2IC4 | 1.4000 | 400 | 35mm3IC6 | 1.3082 | 601 | 26mm4IC8 | 1.2479 |
| 200 | 2eIC4 | 1.4085 | 401 | 44mm3IC6 | 1.3175 | 602 | 3e2m3IC7 | 1.2481 |
| 201 | IC7 | 1.3512 | 402 | 2eIC6 | 1.3140 | | | |

[a] m, methyl; e, ethyl; for example 2mmC3 represent 2,2-dimethyl-propane. [b] Calculated by eq 8


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