Prediction of Standard Enthalpy of Formation by a QSPR Model

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Abstract: The standard enthalpy of formation of 1115 compounds from all chemical groups, were predicted using genetic algorithm-based multivariate linear regression (GA-MLR). The obtained multivariate linear five descriptors model by GA-MLR has correlation coefficient ($R^2 = 0.9830$). All molecular descriptors which have entered in this model are calculated from chemical structure of any molecule. As a result, application of this model for any compound is easy and accurate.

Keywords: QSPR; Enthalpy of formation; GA-MLR.

1. Introduction

Physical and thermodynamic properties data of compounds are needed in the design and operation of industrial chemical processes. Of them, standard enthalpy of formation or standard heat of formation, $\Delta H^\circ$ is an important fundamental physical property of compounds which is defined as change of enthalpy that accompanies the formation of 1 mole of compound in its standard state from its constituent elements in their standard states (the most stable form of the element at 1 atm of pressure and the specified temperature usually 298 K or 25 degrees Celsius). All elements in their standard states (such as hydrogen gas, solid carbon in the form of graphite, etc.) have standard enthalpy of formation of zero, as there is no change involved in their formation.

The standard enthalpy change of formation is used in thermo-chemistry to find the standard enthalpy change of reaction. This is done by subtracting the summation of the standard enthalpies of formation of the reactants from the summation of the standard enthalpies of formation of the products, as shown in the equation below.
where $\Delta H_{\text{reaction}}$, $\sum_p \Delta H_f^p$, and $\sum_r \Delta H_f^r$ are standard enthalpy change of reaction, standard enthalpies of formation of the products, and standard enthalpies of formation of the reactants, respectively.

There are many methods for calculation of $\Delta H_f^*$ in the literature, but of them, only three methods are widely used. These three methods are the Benson method [1], Jobak and Reid method [2], and Constantinou and Gani method [3]. All of these methods are classified in the field of group contribution methods which in these methods, the property of a compound is estimated as a summation of the contributions of simple chemical groups which can occur in the molecular structure. They provide the important advantage of rapid estimates without requiring substantial computational resources.

Application of quantitative structure-property relationship (QSPR) models in prediction and estimation of physical properties of materials is widely developing [4-5]. In QSPR, advanced mathematical methods (Genetic algorithm, neural networks, and etc.) are used to find a relation between property of interest and the basic molecular properties which are obtained solely from the chemical structure of compounds and called "molecular descriptors".

In this study, a new QSPR model for prediction of $\Delta H_f^*$ of 1115 organic compounds is presented. These 1115 compounds belong to all families of materials, as a result the obtained model can be applied for prediction of $\Delta H_f^*$ for any compound.

2. Procedures and Methods

2.1. Data set

Many compilations for $\Delta H_f^*$ have been published in the literature, but of them, we selected the DIPPR 801 [6] compilation for our problem. This compilation has been recommended by AIChE (American Institute of Chemical Engineers). From this compilation, 1115 compounds were selected and $\Delta H_f^*$ of them were extracted from this database.

2.2. Calculation of Molecular Descriptors

In the calculation of molecular descriptors, the optimized chemical structures of compounds are needed. The chemical structures of all 1115 compounds in our data set, were drawn in Hyperchem software [7], and pre-optimized using MM+ mechanical fore field. A more precise optimization was done with PM3 semi empirical method in Hyperchem.

In the next step for all 1115 compounds, molecular descriptors were calculated by Dragon software [8]. Dragon can calculate 1664 molecular descriptors for any chemical structure. After calculating molecular descriptors for all 1115 chemical structures, we must reject non informative descriptors from output of Dragon. First the descriptors with standard deviation lower than 0.0001, have been rejected because these descriptors were near constant. In second step, the descriptors with only one value different from the remaining ones are rejected. In the third step, the pair correlation of each two
descriptors was checked and one of two descriptors with a correlation coefficient equal one (as a threshold value) was excluded. For each pair of correlated descriptors, the one showing the highest pair correlation with the other descriptors rejected from the pool of descriptors.

Finally, the pool of molecular descriptors was reduced by deleting descriptors which could not be calculated for every structure in our data set.

As a result, from the calculated 1664 molecular descriptors, in the first step, only 1477 molecular descriptors remained in the pool of molecular descriptors.

2.3. Methods of calculation and results

In this step, 20% of our database (223 compounds) is randomly removed and entered to test set as an excluded data set. This test set was used in next steps, only for testing the prediction power of obtained model and are not used for developing model. The remaining 80% (892 compounds) of our data set was used for training set.

In this step our problem is to find the best multivariate linear model which has the most accuracy as well as the minimum number of possible molecular descriptors. One of the best algorithms for these types of problems has been proposed by Leardi et al. [9]. In order to perform this algorithm, a program was written based on MATLAB (Mathworks Inc. software). This program finds the best multivariate linear model by genetic algorithm based multivariate linear regression (GA-MLR) which has proposed by Leardi et al. [9] and we have used it to our previous works, successfully [10-12]. The input of this program is the molecular descriptors which have been obtained in previous section and the desired number of parameter of multivariate linear model. The fitness function of our program was the cross validated coefficient. For obtaining the best model, we must consider the effect of increase in the number of molecular descriptors on the increase in the value of the cross validated coefficient. When the cross validated coefficient was quite constant with increasing the number of molecular descriptors, we must stop our search, and the best result has been obtained.

For obtaining the best multivariate linear model, first, we started with one molecular descriptor model and found the best multivariate linear model, then the two molecular descriptors model were tested, and the best multivariate linear two descriptors model was found. This work was repeated and the number of descriptors was increased, till, we found that increase in the number of molecular descriptors does not affect the accuracy of the best model. The best obtained model has six parameters and is presented below:

$$\Delta H_f^* = 50.1688 - 80.52012nSK + 5364546SCBO - 169.21889SCBO - 174.75477nF - 266.57659nHM$$

(2)

where the molecular descriptors of Eq.(2) and their meaning are presented in Table 1.

The statistical parameters of fitting for Eq.(1) are the following: $R^2 = 0.9830$, $F = 10239.02$, $s = 58.541$, $Q^2 = 0.9826$, where $R^2$ is the squared correlation coefficient, $F$ is the Fisher factor, $s$ is the standard deviation, and $Q^2$ is the squared cross validated correlation coefficient. The statistical parameters of coefficients of the Eq. (2) are presented in the Table 2.
Table 1. The molecular descriptors of Eq. (2) and their meaning.

| Variable | Molecular descriptor meaning          |
|----------|---------------------------------------|
| nSK      | Number of non-H atoms                |
| SCBO     | Sum of conventional bond orders (H-depleted) |
| nO       | Number of Oxygen atoms               |
| nF       | Number of Fluorine atoms             |
| nHM      | Number of Heavy atoms                |

Table 2. The values of the constants of Eq. (2) and their statistical interpretations.

| ID | Variable | Regression Coefficient | Errors Regression Coefficient | Confidence Intervals (0.95) | Standard Regression Coefficient |
|----|----------|------------------------|------------------------------|-----------------------------|---------------------------------|
| 0  | intercept| 50.16088267            | 4.075696                     | 0                           | 0                               |
| 1  | nSK      | -80.52012489           | 1.175295                     | -1.081325919                | 3.60196                         |
| 2  | SCBO     | 53.64545627            | 0.9837223                    | 0.858696667                 | 3.593514                        |
| 3  | nO       | -169.2188895           | 1.424115                     | -0.552855974                | 1.061814                        |
| 4  | nF       | -174.7547718           | 1.178939                     | -0.680669749                | 1.047946                        |
| 5  | nHM      | -266.5765885           | 6.857063                     | -0.171389892                | 1.006101                        |

2.4. Validation of Model

There are many validation techniques for checking the validation of the obtained model [13].

Todeschini et al. [13] presented a quick rule for checking the validity of obtained model. This rule compares the multivariate correlation index $K_X$ of X-block of the predictor variables with the multivariate correlation index $K_{XY}$ obtained by the augmented X-block matrix by adding the column of the response variable. This rule says that if $K_{XY}$ is greater than $K_X$, the model is predictive [13]. Obtained values of these two indexes in our problem are $K_X = 31.62$ and $K_{XY} = 40.81$, as a result, with respect to this quick rule, obtained model is predictive ($K_{XY} > K_X$).

Cross-validation technique is the most common validation technique [13]. In this technique each member of our data set is deleted, then, with the other members a model is produced, and the value of the deleted object is predicted. This technique is performed for all members of the data set and finally, a squared cross validated correlation is obtained. In our problem this work was done and the values of squared cross validated correlation ($Q^2$) was 0.9826. The difference between $R^2$ and $Q^2$ is promising and thus validity of this model is confirmed by this technique.

Another validation technique is bootstrap technique [13]. By this technique, validation is performed by randomly generating training sets with sample repetitions and then evaluating the predicted responses of the samples not included in the training set. This work usually repeated thousands of times. After 5000 times repetition of this technique, the parameter $Q_{Boot}^2$ was 0.9823. As can be found,
the difference between the $Q_{\text{boot}}^2$, $Q^2$, and $R^2$ is promising and thus the predictive power of model is confirmed.

Ultimately, the last validation technique which we used was external validation. In this section by means of test set which we had separated from the original data set, the prediction power of the Eq.(2) was checked. The squared cross validated coefficient for the test ($Q_{\text{ext}}^2$) set is 0.9894, which the promising difference between this value and the value of $Q^2$ shows the prediction power of the Eq. (2).

The calculated and DIPPR 801 values of $\Delta H_f^\circ$ for training set are presented in the Table-3. Also, the predicted and DIPPR 801 values of $\Delta H_f^\circ$ for test set are presented in Table 4. The comparison between the results of Eq.(2) and the DIPPR 801 values for training set and test set are shown in the Figure 1.

![Comparison between the results of Eq. (2) for training set and predicted values for training set.](image)

**Figure 1.** Comparison between the results of Eq. (2) for training set and predicted values for training set.

3. Discussion

In the formation of a molecule from its constituent elements, $\Delta H_f^\circ$, is the difference between the enthalpy of this molecule and the elements which conform it. This enthalpy is a result of breaking bonds of the elements in the free form (breaking reaction) and formation of new bonds in the molecule of product (formation reaction). Breaking reaction is endothermic, but the formation reaction is exothermic.

Any thing which can affect the bond properties and strength of the bonds in the molecule can affect the value of $\Delta H_f^\circ$ of that molecule. Of them, the number of atoms and number of the bonds and order
of the bonds and number of non-organic elements (heavy atoms) in a molecule directly affect on the value of $\Delta H_f^\circ$.

Increase in the values of number of atoms in the H-depleted chemical structure of molecule decreases $\Delta H_f^\circ$ of a molecule. Increase in the order of bonds in a molecule increases $\Delta H_f^\circ$. Also the number of atoms which are commonly existed in all molecules such as oxygen and fluorine atoms, and even heavy atoms affect $\Delta H_f^\circ$ of a molecule. Increase in the number of these atoms in a molecule, decreases $\Delta H_f^\circ$ of that molecule.

### Table 3.
The obtained results from Eq. (2) for training set.

| ID | Name                      | $\Delta H_f^\circ$(kJ/mol) | Res  |
|----|---------------------------|-----------------------------|------|
| 1  | n-BUTANE                  | -125.79                     | 14.81|
| 2  | n-HEXANE                  | -198.66                     | 33.93|
| 3  | 3-METHYLPENTANE           | -202.38                     | 37.65|
| 4  | n-HEPTANE                 | -224.05                     | 32.44|
| 5  | 3-METHYLMETHANE           | -226.44                     | 34.83|
| 6  | 3-ETHYLPENTANE            | -224.56                     | 32.95|
| 7  | 2,2-DIMETHYLPENTANE       | -238.28                     | 46.67|
| 8  | 2,3-DIMETHYLPENTANE       | -233.09                     | 41.48|
| 9  | 2,4-DIMETHYLPENTANE       | -234.65                     | 42.99|
| 10 | 3,3-DIMETHYLPENTANE       | -234.18                     | 42.57|
| 11 | 2,2,3-TRIMETHYLBUTANE     | -236.52                     | 44.91|
| 12 | 2-METHYLTEHANE            | -255.01                     | 36.53|
| 13 | 4-METHYLTEHANE            | -251.63                     | 33.15|
| 14 | 3-ETHYLMETHANE            | -250.41                     | 31.93|
| 15 | 2,2-DIMETHYLHEXANE        | -261.88                     | 43.4 |
| 16 | 2,3-DIMETHYLHEXANE        | -252.59                     | 34.11|
| 17 | 2,4-DIMETHYLHEXANE        | -257.02                     | 38.54|
| 18 | 3,3-DIMETHYLHEXANE        | -257.53                     | 39.05|
| 19 | 2-METHYL-3-ETHYLPENTANE   | -249.58                     | 31.1 |
| 20 | 2,2,3-TRIMETHYLHEXANE     | -256.9                      | 38.42|
| 21 | 2,2,4-TRIMETHYLHEXANE     | -259.16                     | 40.68|
| 22 | 2,3,3-TRIMETHYLHEXANE     | -253.51                     | 35.03|
| 23 | 2,3,4-TRIMETHYLHEXANE     | -255.01                     | 36.53|
| 24 | n-NONANE                  | -274.68                     | 29.32|
| 25 | 3,3,5-TRIMETHYLHEXANE     | -304.76                     | 32.53|
| 26 | 2,4,4-TRIMETHYLHEXANE     | -280.2                      | 34.84|
| 27 | 3,3-DIETHYLPENTANE        | -275.39                     | 30.03|
| 28 | 2,2,3,3-TETRAMETHYLHEXANE| -278.28                     | 32.92|
| 29 | 2,2,4,4-TETRAMETHYLHEXANE| -279.99                     | 34.63|
| 30 | SQUALANE                  | -806.3                      | -3.42|
| 31 | n-DECANE                  | -300.62                     | 28.39|
| 32 | 2,2,4,5,5-PENTAMETHYHEXANE| -323.51                    | 51.28|
| 33 | n-UNDECANE                | -326.6                      | 27.49|
| 34 | n-DODECANE                | -352.13                     | 26.15|
| 35 | n-TRIDECANE               | -377.69                     | 24.83|
| 36 | n-TETRADECANE             | -403.25                     | 23.52|
| 37 | n-PENTADECANE             | -428.82                     | 22.22|
| 38 | n-HEXADECANE              | -456.14                     | 22.66|
| 39 | n-OCTADECANE              | -567.14                     | 79.91|
| 40 | n-NONADECANE              | -596.21                     | 82.11|
| 41 | n-HENECOSANE              | -653.45                     | 85.6 |
| 42 | n-DOCOSANE                | -682.07                     | 87.34|
| 43 | n-TRICOSANE               | -710.69                     | 89.09|
| No. | Compound                  | ΔH (kJ/mol) | ΔS (J/mol K) | T° (K) |
|-----|--------------------------|-------------|--------------|--------|
| 44  | n-PENTACOSANE            | -767.93     | -675.35      | 92.58  |
| 45  | n-HEXACOSANE             | -796.55     | -702.23      | 94.32  |
| 46  | n-HEPTACOSANE            | -825.17     | -729.1       | 96.07  |
| 47  | n-OCTACOSANE             | -853.79     | -755.98      | 97.81  |
| 48  | n-NONACOSANE             | -882.41     | -782.85      | 99.56  |
| 49  | 2-METHYLNONANE           | -311.9      | -272.23      | 39.67  |
| 50  | 5-METHYLNONANE           | -310        | -272.23      | 37.77  |
| 51  | 2,2,4,6,8,8-HETAMETHYLNONANE | -476.87  | -433.48      | 43.39  |
| 52  | 3-METHYLOCTANE           | -278.53     | -245.36      | 33.17  |
| 53  | 4-METHYLOCTANE           | -279.6      | -245.36      | 34.24  |
| 54  | 3-ETHYLTEPTANE           | -275.45     | -245.36      | 30.12  |
| 55  | 2,2-DIMETHYLEPTANE       | -288.2      | -245.36      | 42.84  |
| 56  | 3-METHYLUNDECANE         | -355.2      | -325.98      | 29.22  |
| 57  | ETHYL CYCLOPENTANE       | -163.43     | -137.96      | 25.47  |
| 58  | cis-1,2-DIMETHYL CYCLOPENTANE | -165.27 | -137.96      | 27.31  |
| 59  | trans-1,3-DIMETHYL CYCLOPENTANE | -168.07 | -137.96      | 30.11  |
| 60  | n-PROPYL CYCLOPENTANE    | -189.07     | -164.84      | 24.23  |
| 61  | 1-METHYL-1-ETHYL CYCLOPENTANE | -193.8    | -164.84      | 28.96  |
| 62  | n-PROPYLCYCOHEXANE       | -237.4      | -191.71      | 45.69  |
| 63  | ISOPROPYLCYCOHEXANE      | -239.45     | -191.71      | 47.74  |
| 64  | 1,1-DIETHYL CYCLOHEXANE  | -277.11     | -218.59      | 58.52  |
| 65  | n-DECYL CYCLOHEXANE      | -417        | -379.83      | 37.17  |
| 66  | CYCLOHEPTANE             | -156.61     | -137.96      | 18.65  |
| 67  | CYCLOOCTANE              | -167.74     | -164.84      | 2.9    |
| 68  | trans-1,4-DIETHYL CYCLOHEXANE | -266.1    | -218.59      | 47.51  |
| 69  | 2,6-DIMETHYLHEPTANE      | -286.12     | -245.36      | 40.76  |
| 70  | 2,2-DIMETHYL-3-ETHYLHEPTANE | -272.7    | -245.36      | 27.34  |
| 71  | 2,4-DIMETHYL-3-ETHYLHEPTANE | -269.7    | -245.36      | 24.34  |
| 72  | 1-TRIAMCENTE             | -761.6      | -756.08      | 5.52   |
| 73  | 2-METHYL-1-BUTENE        | -60.96      | -84.21       | -23.25 |
| 74  | cis-2-HEXENE             | -80.11      | -111.09      | -30.98 |
| 75  | trans-2-HEXENE           | -85.52      | -111.09      | -25.57 |
| 76  | cis-3-HEXENE             | -78.95      | -111.09      | -32.14 |
| 77  | 2-METHYL-1-PENTENE       | -89.96      | -111.09      | -21.13 |
| 78  | 3-METHYL-1-PENTENE       | -78.16      | -111.09      | -32.93 |
| 79  | 4-METHYL-1-PENTENE       | -80.04      | -111.09      | -31.05 |
| 80  | 2-METHYL-2-PENTENE       | -98.53      | -111.09      | -12.56 |
| 81  | 4-METHYL-1-HEXENE        | -101.5      | -137.96      | -36.46 |
| 82  | 4-METHYL-cis-2-PENTENE   | -87.03      | -111.09      | -24.06 |
| 83  | 4-METHYL-trans-2-PENTENE | -91.55     | -111.09      | -19.54 |
| 84  | 2-ETHYL-1-BUTENE         | -87.11      | -111.09      | -23.98 |
| 85  | 2,3-DIMETHYL-1-BUTENE    | -95.6       | -111.09      | -15.49 |
| 86  | 3,3-DIMETHYL-1-BUTENE    | -88.28      | -111.09      | -22.81 |
| 87  | 2-ETHYL-1-PENTENE        | -109.9      | -137.96      | -28.06 |
| 88  | 1-BRANDENE               | -98.37      | -137.96      | -39.59 |
| 89  | cis-2-HEPTENE            | -105.1      | -137.96      | -32.86 |
| 90  | trans-2-HEPTENE          | -109.5      | -137.96      | -28.46 |
| 91  | trans-3-HEPTENE          | -109.33     | -137.96      | -28.63 |
| 92  | 2-METHYL-1-HEXENE        | -112.6      | -137.96      | -25.36 |
| 93  | 3-ETHYL-1-PENTENE        | -98.49      | -137.96      | -39.47 |
| 94  | 3-METHYL-1-HEXENE        | -101.1      | -137.96      | -36.86 |
| 95  | 3-ETHYL-1-HEXENE         | -124.6      | -164.84      | -40.24 |
| 96  | 2,3,3-TRIMETHYL-1-BUTENE | -117.7      | -137.96      | -20.26 |
| 97  | cis-3-HEPTENE            | -104.35     | -137.96      | -33.61 |
| 98  | 1-OCTENE                 | -122        | -164.84      | -42.84 |
| 99  | 2,4,4-TRIMETHYL-1-PENTENE | -146.15   | -164.84      | -18.69 |
| 100 | 2-ETHYL-1-HEXENE         | -136.42     | -164.84      | -28.42 |
| 101 | 1-NONE       | -148.8      | -191.71      | -42.91 |
| 102 | 1-UNDENECE              | -200.8      | -245.46      | -44.66 |
| 103 | 1-DODECENE              | -226.2      | -272.34      | -46.14 |
| 104 | 1-TRIDECENE             | -253.5      | -299.21      | -45.71 |
| 105 | 1-TETRADECENE           | -280.3      | -326.08      | -45.78 |
| 106 | 1-HEXADECENE            | -329.24     | -379.83      | -50.59 |
|   |   |   |   |
|---|---|---|---|
|107| 1-OCTADECENE| -374.77| -433.58| -58.81|
|108| 6-METHYL-1-HEPTENE| -129.5| -164.84| -35.34|
|109| CYCLOHEXENE| -38.2| -57.44| -19.24|
|110| trans-2-EICOSENE| -446.6| -487.33| -40.73|
|111| trans-2-PENTADECENE| -319.5| -352.96| -33.46|
|112| cis-2-OCTENE| -134.38| -164.84| -30.46|
|113| cis-4-OCTENE| -128.49| -164.84| -36.35|
|114| trans-4-OCTENE| -134.61| -164.84| -30.23|
|115| 1-EICOSENE| -459.21| -487.33| -28.12|
|116| 1-METHYLCYCLOPENTENE| -36.44| -57.44| -21|
|117| 2,3-DIMETHYL-1-HEXENE| -136| -164.84| -28.84|
|118| 1,4-Di-tert-BUTYLBENZENE| -188.9| -165.15| 23.75|
|119| alpha-TOCOPHEROL| -873.4| -879.94| -6.54|
|120| 1,2,3-TRIETHYLBENZENE| -130.32| -111.4| 18.92|
|121| n-HEPTYLBENZENE| -196.36| -165.15| 31.21|
|122| n-DECYLBENZENE| -217.5| -218.9| -1.4|
|123| n-DECYLBENZENE| -258.1| -218.9| 39.2|
|124| n-PENTYLBENZENE| -89.5| -84.52| 4.98|
|125| n-HEXYLBENZENE| -115| -111.4| 3.6|
|126| n-OCTYLBENZENE| -166.1| -165.15| 0.95|
|127| n-NONYLBENZENE| -190.4| -192.02| -1.62|
|128| n-UNDECYLBENZENE| -241.18| -245.77| -4.59|
|129| n-TETRACYLBENZENE| -288.73| -299.52| -10.79|
|130| 2,3-DIMETHYL-2,3-DIPHENYLBUTANE| -311.49| -326.4| -14.91|
|131| 1,1,2,2-TETRAPHENYLETHANE| -264.79| -272.65| -7.86|
|132| TETRAPHENYLMETHANE| -59.68| -58.06| 1.62|
|133| 1,1,2,2-TETRAPHENYLETHANE| -5.01| -4.32| -16.35|
|134| STYRENE| -363.4| -49.75| 53.72|
|135| 1-n-NONYL-NAPHTHALENE| -132.57| -111.76| 20.81|
|136| 1-n-PENTYLNAPHTHALENE| -156.26| -138.27| 17.62|
|137| 1-n-HEXYLNAPHTHALENE| -179.33| -165.25| 14.08|
|138| 1-n-PENTYLNAPHTHALENE| -188.9| -165.15| 31.21|
|139| 1-n-HEXYLNAPHTHALENE| -258.1| -218.9| 39.2|
|140| 1-n-HEXYLNAPHTHALENE| -288.73| -299.52| -10.79|
|141| sec-BUTYLCYCLOHEXANE| -263.7| -218.59| 45.11|
|142| PIMARIC ACID| -634.1| -611.29| 22.81|
|143| SULFUR DIOXIDE| -296.84| -315.26| -18.42|
|144| SULFUR TRIOXIDE| -441.04| -457.7| -16.66|
|145| ACETALDEHYDE| -166.4| -199.68| -33.28|
|146| BUTANAL| -219.2| -226.56| -7.86|
|147| 1,2,3,6-TETRAHYDROBENZALDEHYDE| -201.8| -253.54| -51.74|
|148| 2-METHYL-2-PENTENAL| -239.2| -253.43| -14.23|
|149| 2-ETHYL-2-HEXENAL| -258.1| -307.28| -62.68|
|150| 2,3-DIMETHYL-1,2,3,4-TETRAHYDRONAPHTHALENE| -162.1| -226.76| -64.66|
|151| ACENAPITHALENE| -241.18| -245.77| -4.59|
|152| acenaphthalene| -288.73| -299.52| -10.79|
|153| pimic acid| -363.4| -49.75| 53.72|
|154| 1-n-PENTYLNAPHTHALENE| -132.57| -111.76| 20.81|
|155| 1-n-PENTYLNAPHTHALENE| -156.26| -138.27| 17.62|
|156| 1-n-PENTYLNAPHTHALENE| -179.33| -165.25| 14.08|
|157| 1-n-PENTYLNAPHTHALENE| -188.9| -165.15| 31.21|
|158| 1-n-PENTYLNAPHTHALENE| -201.8| -253.54| -51.74|
|159| 2,3-DIMETHYL-2,3-DIPHENYLBUTANE| -258.1| -218.9| 39.2|
|160| 1,2,3,6-TETRAHYDROBENZALDEHYDE| -162.1| -226.76| -64.66|
|161| 2,3-DIMETHYL-2,3-DIPHENYLBUTANE| -59.68| -58.06| 1.62|
|162| ACENAPITHALENE| -188.9| -165.15| 31.21|
|163| ACENAPITHALENE| -258.1| -218.9| 39.2|
|164| ACENAPITHALENE| -288.73| -299.52| -10.79|
|165| ACENAPITHALENE| -311.49| -326.4| -14.91|
|166| ACENAPITHALENE| -363.4| -49.75| 53.72|
|167| ACENAPITHALENE| -441.04| -457.7| -16.66|
|168| ACENAPITHALENE| -441.04| -457.7| -16.66|
|169| ACENAPITHALENE| -441.04| -457.7| -16.66|
|    | Compound                     |  T1      |  T2      |  T3      |
|----|------------------------------|----------|----------|----------|
| 170| 2-METHYLBUTYRALDEHYDE        | -271.5   | -280.31  | -8.81    |
| 171| 3-METHYLBUTYRALDEHYDE        | -276.5   | -280.31  | -3.81    |
| 172| cis-CROTONALDEHYDE           | -137.7   | -199.79  | -62.09   |
| 173| trans-CROTONALDEHYDE         | -138.7   | -199.79  | -61.09   |
| 174| o-TOLUALDEHYDE               | -113.18  | -146.35  | -33.17   |
| 175| p-HYDROXYBENZALDEHYDE        | -310.82  | -315.57  | -4.75    |
| 176| TEREPHTHALDEHYDE             | -243.43  | -288.8   | -45.37   |
| 177| 2-METHYL OCTANAL             | -370.2   | -387.8   | -17.6    |
| 178| METHYL ETHYL KETONE          | -273.3   | -253.43  | 19.87    |
| 179| METHYL ISOBUTYL KETONE       | -328.4   | -307.18  | 21.22    |
| 180| 3-METHYL-2-PENTANONE         | -323.8   | -307.18  | 16.62    |
| 181| 3-HEPTANONE                  | -346.2   | -334.06  | 14.54    |
| 182| 4-HEPTANONE                  | -346.2   | -334.06  | 12.14    |
| 183| 3-HXANONE                    | -320.2   | -307.18  | 13.02    |
| 184| 2-HXANONE                    | -322.01  | -307.18  | 14.83    |
| 185| Mesityl OXIDE                | -238.14  | -253.54  | -15.4    |
| 186| 3,3-DIMETHYL-2-BUTANONE      | -328.6   | -307.18  | 21.42    |
| 187| DISOBUTYL KETONE             | -408.5   | -387.8   | 20.7     |
| 188| DISOPROPYL KETONE            | -352.92  | -334.06  | 18.86    |
| 189| 2-PYRROLIDONE                | -266.04  | -226.66  | 39.38    |
| 190| N-METHYL-2-PYRROLIDONE       | -262.2   | -253.54  | 8.66     |
| 191| ETHYL ISOAMYL KETONE         | -374.4   | -360.93  | 13.47    |
| 192| 5-NONANONE                   | -398.24  | -387.8   | 10.44    |
| 193| 2-NONANONE                   | -396.8   | -387.8   | 9        |
| 194| ACETYLACETONE                | -423.8   | -422.75  | 1.05     |
| 195| CYCLOPENTANONE               | -235.7   | -226.66  | 9.04     |
| 196| CYCLOHEXANONE                | -271.2   | -253.54  | 17.66    |
| 197| 2-OCTANONE                   | -372.7   | -360.93  | 11.77    |
| 198| BENZOPHENONE                 | -37.3    | -66.14   | -28.84   |
| 199| ACETOPHENONE                 | -142.5   | -146.35  | -3.85    |
| 200| beta-PROPIONOLCTONE          | -329.9   | -369     | -39.1    |
| 201| 2-CYCLOHEXYL CYCLOHEXANONE   | -390.98  | -361.14  | 29.84    |
| 202| METHANOL                     | -239.1   | -226.45  | 12.65    |
| 203| ETHANOL                      | -276.98  | -253.33  | 23.65    |
| 204| 1-PROANOL                    | -302.6   | -280.2   | 22.4     |
| 205| ISOPROANOL                   | -318.1   | -280.2   | 37.9     |
| 206| 1-BUTANOL                    | -327.2   | -307.08  | 20.12    |
| 207| 2-BUTANOL                    | -324.6   | -307.08  | 35.52    |
| 208| 2-METHYL-2-PROANOL           | -365.9   | -307.08  | 58.82    |
| 209| 1-PENTANOL                   | -351.6   | -333.95  | 17.65    |
| 210| 2-PENTANOL                   | -365.2   | -333.95  | 31.25    |
| 211| 2-METHYL-1-BUTANOL           | -356.6   | -333.95  | 22.65    |
| 212| 2,2-DIMETHYL-1-PROANOL       | -382.01  | -333.95  | 48.06    |
| 213| 1-HXANOL                     | -377.5   | -360.83  | 16.67    |
| 214| 2-HXANOL                     | -392     | -360.83  | 31.17    |
| 215| 3-METHYL-1-PENTANOL          | -380.9   | -360.83  | 20.07    |
| 216| 3-PENTANOL                   | -370.33  | -333.95  | 36.38    |
| 217| 2-ETHYL-1-HXANOL             | -432.8   | -414.58  | 18.22    |
| 218| 2-METHYL-1-HXANOL            | -404.5   | -387.7   | 16.8     |
| 219| 3-METHYL-1-BUTANOL           | -356.4   | -333.95  | 22.45    |
| 220| 1-HEPTANOL                   | -403.3   | -387.7   | 15.6     |
| 221| 1-NONANOL                    | -453.6   | -441.45  | 12.15    |
| 222| 1-DECANOL                    | -478.1   | -468.32  | 9.78     |
| 223| 1-UNDECANOL                  | -504.8   | -495.2   | 9.6      |
| 224| 8-METHYL-1-NONANOL           | -483.13  | -468.32  | 14.81    |
| 225| 1-DODECANOL                  | -528.5   | -522.07  | 6.43     |
| 226| 1-TRIDECANOL                 | -599.4   | -548.95  | 50.45    |
| 227| 1-TETRADECANOL               | -628.18  | -575.82  | 52.36    |
| 228| 1-PENTADECANOL               | -658.2   | -602.7   | 55.5     |
| 229| 1-HEPTADECANOL               | -722.85  | -656.45  | 66.4     |
| 230| 2-ETHYL-1-BUTANOL            | -382.41  | -360.83  | 21.58    |
| 231| 1-METHYL CYCLOHEXANOL        | -388.17  | -334.06  | 54.11    |
| 232| cis-2-METHYL CYCLOHEXANOL    | -390.2   | -334.06  | 56.14    |
| No. | Compound                        | ΔH (kJ/mol) | ΔG (kJ/mol) | ΔS (kJ/mol) |
|-----|--------------------------------|-------------|-------------|-------------|
| 233 | cis-3-METHYLCYCLOHEXANOL        | -416.1      | -334.06     | 82.04       |
| 234 | trans-3-METHYLCYCLOHEXANOL      | -394.4      | -334.06     | 60.34       |
| 235 | cis-4-METHYLCYCLOHEXANOL        | -413.2      | -334.06     | 79.14       |
| 236 | trans-4-METHYLCYCLOHEXANOL      | -433.3      | -334.06     | 99.24       |
| 237 | AGATHADIOL                      | -685.7      | -718.58     | -32.88      |
| 238 | alpha-TERPINEOL                 | -316.7      | -361.03     | -44.33      |
| 239 | 2-BUTYL-NONAN-1-OL              | -540.1      | -548.95     | -8.85       |
| 240 | TETRAHYDROFURFURYL ALCOHOL      | -435.7      | -476.4      | -40.7       |
| 241 | 2-PHENYL-2-PROPanOL             | -244.43     | -226.87     | 17.56       |
| 242 | 2-BUTYL-OCTAN-1-OL              | -512.2      | -522.07     | -9.87       |
| 243 | 2,6-XYLENOL                     | -237.4      | -199.99     | 37.41       |
| 244 | BENZYL ALCOHOL                  | -160.71     | -173.12     | -12.41      |
| 245 | m-CRESOL                        | -194        | -173.12     | 20.88       |
| 246 | o-ETHYLPHENOL                   | -208.82     | -199.99     | 8.83        |
| 247 | p-HYDROQUINONE                  | -371.1      | -342.34     | 28.76       |
| 248 | p-ETHYLPHENOL                   | -224.39     | -199.99     | 24.4        |
| 249 | p-tert-BUTYLPHENOL              | -276.66     | -253.74     | 22.92       |
| 250 | BISPHENOL A                     | -368.5      | -369.63     | -1.13       |
| 251 | NONYLPHENOL                     | -387.33     | -388.12     | -0.79       |
| 252 | ETHYLENE GLYCOL                 | -460        | -449.42     | 10.58       |
| 253 | DIETHYLENE GLYCOL               | -628.5      | -699.26     | -70.76      |
| 254 | TETRAETHYLENE GLYCOL            | -981.7      | -1198.95    | -217.25     |
| 255 | 1,2-PROPYLENE GLYCOL            | -499.99     | -476.3      | 23.69       |
| 256 | 1,3-PROPYLENE GLYCOL            | -480.8      | -476.3      | 4.5         |
| 257 | DIPROPYLENE GLYCOL              | -718.46     | -753.01     | -34.55      |
| 258 | 2-METHYL-1,3-PROPANEDIOL        | -505.9      | -503.17     | 2.73        |
| 259 | 1,2-BUTANEDIOL                  | -523.6      | -503.17     | 20.43       |
| 260 | 1,3-BUTANEDIOL                  | -501        | -503.17     | -2.17       |
| 261 | HEXYLENE GLYCOL                 | -602.92     | -556.92     | 46          |
| 262 | GLYCEROL                        | -669.6      | -672.39     | -2.79       |
| 263 | p-tert-BUTYLCATECHOL             | -474        | -449.84     | 24.16       |
| 264 | 2,2,4-TRIMETHYL-1,3-PENTANEDIOL | -497.18     | -610.67     | -113.49     |
| 265 | 2-METHYL-1,3-PENTANEDIOL        | -577.5      | -556.92     | 20.58       |
| 266 | 2,3-BUTANEDIOL                  | -541.5      | -503.17     | 38.33       |
| 267 | cis-2-BUTENE-1,4-DIOL           | -372.9      | -449.52     | -76.62      |
| 268 | trans-2-BUTENE-1,4-DIOL         | -401.6      | -449.52     | -47.92      |
| 269 | 1,5-PENTANEDIOL                 | -531.49     | -530.05     | 1.44        |
| 270 | 1,6-HEXANEDIOL                  | -583.86     | -556.92     | 26.94       |
| 271 | 1,2-BENZENEDIOL                 | -354.1      | -342.34     | 11.76       |
| 272 | 1,3-BENZENEDIOL                 | -368        | -342.34     | 25.66       |
| 273 | PENTAERYTHRITOL                 | -920.6      | -922.23     | -1.63       |
| 274 | TRIMETHYLOLPROPAINE             | -751.61     | -753.01     | -1.4        |
| 275 | 1,2,3-BENZENETRIOL              | -551.1      | -538.43     | 12.67       |
| 276 | SORBITOL                        | -1354.2     | -1341.29    | 12.91       |
| 277 | FORMIC ACID                     | -425.5      | -368.9      | 56.6        |
| 278 | ACETIC ACID                     | -484.5      | -395.78     | 88.72       |
| 279 | PROPIONIC ACID                  | -508.5      | -422.65     | 85.85       |
| 280 | n-DECANOIC ACID                 | -713.7      | -610.77     | 102.93      |
| 281 | OXALIC ACID                     | -829.7      | -734.32     | 95.38       |
| 282 | n-BUTYRIC ACID                  | -533.8      | -449.52     | 84.28       |
| 283 | n-PENTANOIC ACID                | -558.7      | -476.4      | 82.3        |
| 284 | n-NONANOIC ACID                 | -661.8      | -583.9      | 77.9        |
| 285 | ISOBUTYRIC ACID                 | -531        | -449.52     | 81.48       |
| 286 | ISOVALERIC ACID                 | -561.6      | -476.4      | 85.2        |
| 287 | n-HEXANOIC ACID                 | -583.8      | -503.27     | 80.53       |
| 288 | 2-METHYLMETHANOIC ACID          | -613.9      | -530.15     | 83.75       |
| 289 | 1,4-CYCLOHEXANEDICARBOXYLIC ACID| -998.5      | -841.92     | 156.58      |
| 290 | n-OCTANOIC ACID                 | -636.8      | -557.02     | 79.78       |
| 291 | n-UNDECANOIC ACID               | -735.9      | -637.65     | 98.25       |
| 292 | CYCLOPENTYLACETIC ACID          | -551.73     | -476.5      | 75.23       |
| 293 | DILACTIC ACID                   | -1122.8     | -1037.91    | 84.89       |
| 294 | n-DODECANOIC ACID               | -774.6      | -664.52     | 110.08      |
| 295 | n-HEXADECANOIC ACID             | -891.5      | -772.02     | 119.48      |
| No. | Chemical Name                      | ΔH°  | ΔS°  | ΔfG°  |
|-----|-----------------------------------|-------|------|-------|
| 296 | trans-CROTONIC ACID               | -446.23 | -395.88 | 50.35 |
| 297 | STEARIC ACID                      | -948.00 | -825.77 | 122.23 |
| 298 | ACRYLIC ACID                      | -383.88 | -369.00 | 14.88 |
| 299 | OLEIC ACID                        | -802.49 | -772.12 | 30.37 |
| 300 | LINOLEIC ACID                     | -674.04 | -718.48 | -44.44 |
| 301 | SALICYLIC ACID                    | -589.90 | -511.66 | 78.24 |
| 302 | ADIPIC ACID                       | -994.30 | -841.82 | 152.48 |
| 303 | MALEIC ACID                       | -789.40 | -734.42 | 53.30 |
| 304 | TEREPHthalic ACID                 | -816.18 | -680.98 | 135.20 |
| 305 | ACETIC ANHYDRIDE                  | -624.40 | -591.97 | 32.43 |
| 306 | PROPIONIC ANHYDRIDE               | -679.10 | -645.72 | 33.38 |
| 307 | BUTYRIC ANHYDRIDE                 | -719.12 | -699.47 | 19.65 |
| 308 | PALUSTRIC ACID                    | -852.40 | -664.94 | 187.46 |
| 309 | SUCCINIC ANHYDRIDE                | -607.80 | -538.33 | 69.47 |
| 310 | GLUTARIC ANHYDRIDE                | -618.50 | -565.20 | 53.30 |
| 311 | PHthalic ANHYDRIDE                | -460.10 | -431.24 | 28.86 |
| 312 | MALEIC ANHYDRIDE                  | -469.80 | -484.68 | -14.88 |
| 313 | TRIMELLITIC ANHYDRIDE             | -894.81 | -796.66 | 98.15 |
| 314 | METHYL FORMATE                    | -386.10 | -395.78 | -9.68 |
| 315 | n-PROPyl FORMATE                  | -445.20 | -449.52 | -4.32 |
| 316 | n-BUTyl FORMATE                   | -469.20 | -476.40 | -7.20 |
| 317 | ISOBUTYL FORMATE                  | -475.87 | -476.40 | -0.53 |
| 318 | n-PENTyl FORMATE                  | -493.28 | -503.27 | -9.99 |
| 319 | n-OCTyl FORMATE                   | -566.45 | -583.90 | -17.45 |
| 320 | n-NONyl FORMATE                   | -588.93 | -610.77 | -21.84 |
| 321 | n-DECyl FORMATE                   | -613.73 | -637.65 | -23.92 |
| 322 | VINYL FORMATE                     | -293.36 | -369.00 | -75.64 |
| 323 | ETHYL ACETATE                     | -478.80 | -449.52 | 29.28 |
| 324 | n-PROPyl ACETATE                  | -504.32 | -476.40 | 27.92 |
| 325 | n-BUTyl ACETATE                   | -529.20 | -503.27 | 25.93 |
| 326 | ISOBUTyl ACETATE                  | -536.06 | -503.27 | 32.79 |
| 327 | n-PENTyl ACETATE                  | -558.69 | -530.15 | 28.54 |
| 328 | ALLyl ACETATE                     | -386.30 | -422.75 | -36.45 |
| 329 | ISOPROPyl ACETATE                 | -518.80 | -476.40 | 42.40 |
| 330 | sec-BUTyl ACETATE                 | -544.04 | -503.27 | 40.77 |
| 331 | VINYL ACETATE                     | -349.70 | -395.88 | -46.18 |
| 332 | METHYL PROPIONATE                 | -463.30 | -449.52 | 13.78 |
| 333 | ETHYL PROPIONATE                  | -502.70 | -476.40 | 26.30 |
| 334 | n-PROPyl PROPIONATE               | -527.50 | -503.27 | 24.23 |
| 335 | n-BUTyl PROPIONATE                | -549.90 | -530.15 | 19.75 |
| 336 | VINYL PROPIONATE                  | -385.46 | -422.75 | -37.29 |
| 337 | ETHYL n-BUTYRATE                  | -514.63 | -503.27 | 11.36 |
| 338 | n-PROPyl ISOBYTyrATE              | -564.50 | -530.15 | 34.35 |
| 339 | METHYL ACRYLATE                   | -362.20 | -395.88 | -33.68 |
| 340 | ETHYL ACRYLATE                    | -379.59 | -422.75 | -43.16 |
| 341 | n-PROPyl ACRYLATE                 | -407.17 | -449.63 | -42.46 |
| 342 | n-BUTyl NONOATE                   | -697.78 | -691.40 | 6.38 |
| 343 | n-BUTyl VALERATE                  | -613.30 | -583.90 | 29.40 |
| 344 | ETHYL ISOVALERATE                 | -570.90 | -530.15 | 40.75 |
| 345 | METHYL METHACRYLATE               | -399.13 | -422.75 | -23.62 |
| 346 | ETHYL METHACRYLATE                | -421.34 | -449.63 | -28.29 |
| 347 | n-PROPyl METHACRYLATE             | -446.70 | -476.50 | -29.80 |
| 348 | DIOCTYL PHthalATE                 | -1084.10 | -1110.98 | 26.88 |
| 349 | DIISOOCYTL PHthalATE              | -1087.30 | -1110.98 | 23.68 |
| 350 | 1,2-BENZENEDICARBOXYLIC ACID, HEPTYL, NONYL ESTER | -1085.00 | -1110.98 | 25.98 |
| 351 | n-PENTyl ACETATE                 | -553.00 | -530.15 | 22.85 |
| 352 | 2-ETHYLHEXYL ACETATE             | -627.99 | -610.77 | 17.22 |
| 353 | BENZYL ACETATE                   | -368.80 | -369.32 | -0.52 |
| 354 | ISOBUTyl ISOBYTyrATE              | -594.07 | -557.02 | 37.05 |
| 355 | n-PENTyl ISOBYLATER              | -644.74 | -610.77 | 33.97 |
| 356 | METHYL OLEATE                    | -734.50 | -799.00 | 64.50 |
| 357 | n-HEXYL ACETATE                  | -577.90 | -557.02 | 20.88 |
|   |   |   |   |
|---|---|---|---|
| 358 | n-BUTYL BENZOATE | -429.06 | -423.07 | 5.99 |
| 359 | n-HEPTYL ACETATE | -602.67 | -583.9 | 18.77 |
| 360 | n-OCTYL ACETATE | -628.25 | -610.77 | 17.48 |
| 361 | n-DECYL ACETATE | -679.25 | -664.52 | 14.73 |
| 362 | DISODOECYL PHTHALATE | -1196.9 | -1218.48 | -21.58 |
| 363 | METHYL SALICYLATE | -531.79 | -538.54 | -6.75 |
| 364 | DI-n-NONYL PHTHALATE | -1134.8 | -1164.73 | -29.93 |
| 365 | DI-n-PROPYL PHTHALATE | -811.89 | -842.23 | -30.34 |
| 366 | DISOBUTYL PHTHALATE | -890.0 | -895.98 | -5.98 |
| 367 | n-OCTYL ACETATE | -628.25 | -610.77 | 17.48 |
| 368 | DI-n-DECYL PHTHALATE | -1197.0 | -1218.48 | -21.48 |
| 369 | DI-n-UNDECYL PHTHALATE | -1248.0 | -1325.98 | -77.98 |
| 370 | DI-n-HEXYL PHTHALATE | -987.8 | -1003.48 | -15.68 |
| 371 | DIMETHYL TEREPTHALATE | -732.6 | -734.73 | -2.13 |
| 372 | DI-n-OCTYL TEREPTHALATE | -1181.2 | -1110.98 | 70.22 |
| 373 | n-BUTYL STEARATE | -978.16 | -933.27 | 44.89 |
| 374 | DIBUTYL SEBACATE | -1156.7 | -1164.31 | -7.61 |
| 375 | n-BUTYL n-BUTYRATE | -575.39 | -557.02 | 18.37 |
| 376 | METHYL BENZOATE | -343.5 | -342.44 | 1.06 |
| 377 | ETHYL BENZOATE | -379.91 | -369.32 | 10.59 |
| 378 | DIETHYL CARBONATE | -682.65 | -672.49 | 10.16 |
| 379 | DIETHYL OXALATE | -806.28 | -841.82 | -35.54 |
| 380 | DIETHYL MALONATE | -838.02 | -868.69 | -30.67 |
| 381 | ISOPROPYL MYRISTATE | -820.33 | -798.9 | 21.43 |
| 382 | 1,2-BENZENE DICARBOXYLIC ACID, HEPTYL, UNDECYL ESTER | -1137.0 | -1164.73 | -27.73 |
| 383 | DIMETHYL ETHER | -184.1 | -253.33 | -69.23 |
| 384 | DIETHYL ETHER | -279.4 | -307.08 | -27.68 |
| 385 | DIISOPROPYL ETHER | -351.5 | -360.83 | -9.33 |
| 386 | METHYL tert-BUTYL ETHER | -377.9 | -414.58 | -36.68 |
| 387 | METHYL ETHYL ETHER | -216.4 | -280.2 | -63.8 |
| 388 | METHYL n-PROPYL ETHER | -265.89 | -307.08 | -41.19 |
| 389 | METHYL ISOBUTYL ETHER | -290.6 | -333.95 | -43.35 |
| 390 | ETHYL PROPYL ETHER | -303.59 | -333.95 | -30.36 |
| 391 | 1,4-DIOXANE | -355.1 | -449.52 | -94.42 |
| 392 | TRIOXANE | -522.5 | -618.74 | -96.24 |
| 393 | DI-n-HEXYL ETHER | -481.96 | -522.07 | -40.11 |
| 394 | METHYL n-BUTYL ETHER | -290.6 | -333.95 | -43.35 |
| 395 | ETHYL n-PENTYL ETHER | -303.59 | -360.83 | -30.36 |
| 396 | 1-METHYL-3-(METHYLETHOXY)BENZENE | -221.6 | -253.74 | -32.14 |
| 397 | 1,1-DIMETHOXYETHANE | -420.1 | -503.17 | -83.07 |
| 398 | 2,5-DIHYDROFURAN | -141.36 | -199.79 | -58.43 |
| 399 | TETRAHYDROFURAN | -216.19 | -253.43 | -37.24 |
| 400 | 1-tert-BUTOXY-2-[2-(tert-BUTOXY)PROPOXY]PROPANE | -810.3 | -968.01 | -157.71 |
| Substance                      | T1   | T2    | T3    |
|-------------------------------|------|-------|-------|
| 1,2-DIMETHOXYPROpane         | -422.3 | -530.05 | -107.75 |
| sec-BUTYL-tert-BUTYL ETHER   | -417.5 | -414.58 | 2.92   |
| ISOBUTYL-tert-BUTYL ETHER    | -407  | -414.58 | -7.58  |
| 1,4-DICHLORO-trans-2-BUTENE  | -112.53 | -111.09 | 1.44   |
| HEXACHLOROETHANE             | -202.8 | -218.48 | -15.68 |
| 1,1,1,2-TETRACHLOROETHANE    | -191  | -164.73 | 26.27  |
| 1,1,2,2-TETRACHLOROETHANE    | -194.6 | -164.73 | 29.87  |
| HEXACHLOROCYCLOPENTADIENE    | -159.78 | -138.17 | 21.61  |
| PENTACHLOROETHANE            | -187.6 | -191.61 | -4.01  |
| 3,4-DICHLORO-1-BUTENE        | -106.91 | -111.09 | -4.18  |
| DICHLORODIFLUOROMETHANE      | -491.62 | -487.37 | 4.25   |
| HEXACHLOROCYCLOPENTADIENE    | -159.78 | -138.17 | 21.61  |
| 1,4-DICHLOROTETRAFLUOROETHANE| -916.3 | -917.5  | -1.2   |
| 1,2-DIBROMOTETRAFLUOROETHANE | -807.1 | -917.5  | -110.4 |
| METHYL FLUORIDE              | -234.3 | -231.99 | 2.31   |
| DIFLUOROMETHANE              | -452.3 | -433.62 | 18.68  |
| TRIFLUOROMETHANE             | -697.05 | -662.12 | 61.8   |
| CARBON TETRAFLUORIDE         | -933.15 | -836.88 | 96.27  |
| ETHYL FLUORIDE               | -264.4 | -258.86 | 5.54   |
| 1,1,1-TRIFLUOROETHANE        | -736.4 | -662.12 | 74.28  |
| DECAFLUOROBUTANE             | -2149.7 | -2127.28 | 22.42 |
| PERFLUORO-n-DECANE           | -4710  | -4708.08 | 1.92   |
| 1,1-DIFLUOROETHYLENE         | -328.96 | -406.85 | -77.89 |
| TETRAFLUOROETHYLENE          | -658.56 | -810.11 | -151.55 |
| BROMOFLUOROMETHANE           | -424.9 | -460.49 | -35.59 |
| 1,1-DIFLUOROETHANE           | -497  | -460.49 | 36.51  |
| 1-BROMOPROPAINE              | -121.8 | -110.98 | 10.82  |
| 1-BROMOBUTANE                | -143.8 | -137.86 | 5.94   |
| 1-BROMOHEPTANE               | -218.4 | -218.48 | -0.08  |
| 1,2-DIBROMOETHANE            | -79.2  | -110.98 | -31.78 |
| 1,1,1-TRICHLOROTRIFLUOROETHANE| -822  | -742.75 | 79.25  |
| ISOPROPYL IODIDE             | -74.8  | -110.98 | -36.18 |
| 2,2-DICHLORO-1,1,1-TRIFLUOROETHANE | -770.3 | -715.87 | 54.43  |
| HEXAFLUOROPROPYLENE          | -1079  | -1240.24 | -161.24 |
| 2-METHYL-2-AMINOButANE       | -171.4 | -164.73 | 6.67   |
| Di-n-PROPYLAMINE             | -566.11 | -191.61 | -35.5   |
| DIETHYLAMINE                 | -103.7 | -137.86 | -34.16 |
| n-PROPYLAMINE                | -101.47 | -110.98 | 9.51   |
| n-PENTYLAMINE                | -152.62 | -164.73 | -12.11 |
| ISOBUTYLAMINE                | -132.6 | -137.86 | -5.26  |
| DISOBUTYLAMINE               | -218.5 | -245.36 | -26.86 |
| PYRROLE                      | 63.11  | 49.9   | -13.21 |
| METHYL DIETHANOLAMINE        | -473.77 | -556.92 | -83.15 |
| DIETHANOLAMINE               | -493.8 | -530.05 | -36.25 |
| TRIETHANOLAMINE              | -667.35 | -779.89 | -112.54 |
| sec-BUTYLAMINE               | -137.49 | -137.86 | -0.37  |
| tert-BUTYLAMINE              | -150.6 | -137.86 | 12.74  |
| CYCLOHEXYLAMINE              | -147.7 | -137.96 | 9.74   |
| HEXAMETHYLDIENAMINE          | -192.42 | -218.48 | -26.06 |
| DISOPROPYLAMINE              | -178.5 | -191.61 | -13.11 |
| Di-n-BUTYLAMINE              | -206  | -245.36 | -39.36 |
| PIPERIDINE                   | -86.4  | -111.09 | -24.69 |
| QUINOLINE                    | 141.22 | 130.11 | -11.11 |
| FORMANILIDE                  | -151.46 | -146.35 | 5.11   |
| 1,2-PROPANEDIAMINE           | -97.8  | -137.86 | -40.06 |
| N-METHYLPYRROLE              | 62.38  | 23.03  | -39.35 |
| DIPHENYLAMINE                | 130   | 76.31  | -53.69 |
| HYDRACRYLONITRILE            | -161.2 | -199.79 | -38.59 |
| HYDROGEN CYANIDE             | 108.19 | 50.06  | -58.13 |
| ACETONITRILE                 | 40.56  | 23.18  | -17.38 |
| METHACRYLONITRILE            | 64.78  | 23.08  | -41.7  |
|   |   |   |   |
|---|---|---|---|
| 483 | VALERONITRILE | -33.1 | -57.44 | -24.34 |
| 484 | BENZONITRILE | 163.18 | 103.39 | -59.79 |
| 485 | PYRIDINE | 100.2 | 49.85 | -50.35 |
| 486 | HEXAMETHYLENEIMINE | -103.82 | -137.96 | -34.14 |
| 487 | 2-METHYLPYRIDINE | 56.7 | 22.97 | -33.73 |
| 488 | tert-BUTYL MERCAPTAN | -140.5 | -191.61 | 2.64 |
| 489 | ISOBUTYL MERCAPTAN | -120.1 | -164.73 | 4.16 |
| 490 | sec-BUTYL MERCAPTAN | -248.66 | -272.23 | -23.57 |
| 491 | CYCLOHEXYL MERCAPTAN | -244.27 | -245.36 | -0.99 |
| 492 | METHYL ETHYL SULFIDE | -91.6 | -110.98 | -19.38 |
| 493 | METHYL n-PROPYL SULFIDE | -118.5 | -137.86 | -19.36 |
| 494 | METHYL t-BUTYL SULFIDE | -157.1 | -164.73 | -7.63 |
| 495 | DI-n-PROPYL SULFIDE | -169.9 | -191.61 | -21.71 |
| 496 | ETHYL n-OCTYL SULFIDE | -273.3 | -299.11 | -25.81 |
| 497 | METHYL ETHER | 80.2 | 49.9 | -30.3 |
| 498 | THIOPHENE | 80.2 | 49.9 | -30.3 |
| 499 | TETRAHYDROTHIOPHENE | 59.26 | 22.87 | -36.39 |
| 500 | DIETHYL DISULFIDE | 59.26 | 22.87 | -36.39 |
| 501 | UNDECYL MERCAPTAN | 327.18 | 352.86 | -25.68 |
| 502 | n-DODECYL MERCAPTAN | 327.18 | 352.86 | -25.68 |
| 503 | n-PENTYL MERCAPTAN | 327.18 | 352.86 | -25.68 |
| 504 | DICYCLOHEXYL SULFIDE | 327.18 | 352.86 | -25.68 |
| 505 | TRICHLOROACETYL CHLORIDE | 327.18 | 352.86 | -25.68 |
| 506 | TRICHLOROACETYL CHLORIDE | 327.18 | 352.86 | -25.68 |
| 507 | BENZYL CHLORIDE | 327.18 | 352.86 | -25.68 |
| 508 | p-CHLOROBENZOTRIFLUORIDE | 327.18 | 352.86 | -25.68 |
| 509 | 2,4-DICHLOROBENZOTRIFLUORIDE | 327.18 | 352.86 | -25.68 |
| 510 | FLUOROBENZENE | 327.18 | 352.86 | -25.68 |
| 511 | 3-CHLORO-1,2-PROPANEDIOL | 327.18 | 352.86 | -25.68 |
| 512 | 1,3-DICHLORO-2-PROPANOL | 327.18 | 352.86 | -25.68 |
| 513 | DI(2-CHLOROETHYL)ETHER | 327.18 | 352.86 | -25.68 |
| 514 | 3-(METHYLMERCAPTO)PROPANAL | 327.18 | 352.86 | -25.68 |
| 515 | GLYCINE | 327.18 | 352.86 | -25.68 |
| 516 | 4-METHOXYPHENYLACETIC ACID | 327.18 | 352.86 | -25.68 |
| 517 | TRIFLUOROCETIC ACID | 327.18 | 352.86 | -25.68 |
| 518 | ACETALDOL | 327.18 | 352.86 | -25.68 |
| 519 | FURFURAL | 327.18 | 352.86 | -25.68 |
| 520 | ACETOMETHOXANE | 327.18 | 352.86 | -25.68 |
| 521 | ETHYLENE GLYCOL DIACRYLATE | 327.18 | 352.86 | -25.68 |
| 522 | PROPYLENE GLYCOL MONOMETHYL ETHER | 327.18 | 352.86 | -25.68 |
| 523 | DIACRYLATE | 327.18 | 352.86 | -25.68 |
| 524 | ACETATE | 327.18 | 352.86 | -25.68 |
| 525 | ETHYL GLYCOL DIACRYLATE | 327.18 | 352.86 | -25.68 |
| 526 | PROPYLENE GLYCOL MONOMETHYL ETHER | 327.18 | 352.86 | -25.68 |
| 527 | ACETATE | 327.18 | 352.86 | -25.68 |
| No. | Compound                     | ΔH° (kJ/mol) | ΔS° (kJ/mol K) | ΔG° (kJ/mol) |
|-----|------------------------------|--------------|---------------|-------------|
| 545 | SULFURIC ACID                | -813.99      | -707.44       | 106.55      |
| 546 | SULFUR HEXAFLUORIDE         | -1220.5      | -1240.14      | -19.64      |
| 547 | SULFURYL CHLORIDE            | -394.1       | -369          | 25.1        |
| 548 | THIONYL CHLORIDE             | -245.6       | -226.56       | 19.04       |
| 549 | HEXAMETHYLCYCLOTRISILOXANE   | -1622        | -1579.72      | 42.28       |
| 550 | DODECAMETHYLPENTASILOXANE    | -2621        | -2577.61      | 43.39       |
| 551 | METHYL VINYL DICHLOROSILANE  | -380.8       | -377.66       | 3.14        |
| 552 | [3-(MERCAPTO)PROPYL]TRIETHOXYSILANE | -1054 | -1153.96     | -99.96      |
| 553 | 3-(TRIMETHOXYSILYL)-1-PROPANETHIOL | -933.1 | -1073.34     | -140.24     |
| 554 | OCTAMETHYLCYCLOTETASILOXANE  | -2195        | -2123.02      | 71.98       |
| 555 | GLUTARALDEHYDE               | -365.87      | -422.75       | -56.88      |
| 556 | n-TRIACONTANE                | -911.03      | -809.72       | 101.31      |
| 557 | n-DOTRIACONTANE              | -969.93      | -863.47       | 106.46      |
| 558 | 3-OCTANONE                   | -371.8       | -360.93       | 10.87       |
| 559 | 4-OCTANONE                   | -373.1       | -360.93       | 12.17       |
| 560 | n-HEXATRIACONTANE            | -1082.8      | -970.97       | 111.83      |
| 561 | 2-CYCLOHEXENE-1-ONE          | -170.9       | -199.89       | -28.99      |
| 562 | 2,3-DIMETHYLOCTANE           | -304.31      | -272.23       | 32.08       |
| 563 | 2,4-DIMETHYLOCTANE           | -307.95      | -272.23       | 35.72       |
| 564 | 2,5-DIMETHYLOCTANE           | -308.42      | -272.23       | 36.19       |
| 565 | 2,6-DIMETHYLOCTANE           | -307.95      | -272.23       | 35.72       |
| 566 | m-ETHYLPHENOL                | -214.3       | -199.99       | 14.31       |
| 567 | 2-PHENYLETHANOL              | -181.61      | -199.99       | -18.38      |
| 568 | 2,6-DIMETHYL-4-HEPTANOL      | -469.54      | -441.45       | 28.09       |
| 569 | 1-PHENYL-1-PROPANOL          | -219.78      | -226.87       | -7.09       |
| 570 | 3-PHENYL-1-PROPANOL          | -217.9       | -226.87       | -8.97       |
| 571 | beta-CHOLESTEROL             | -726.92      | -656.97       | 69.95       |
| 572 | alpha-METHYL BENZYL ALCOHOL  | -197.43      | -199.99       | -2.56       |
| 573 | o-TOLUALCOHOL                | -206.7       | -199.99       | 6.71        |
| 574 | m-TOLUALCOHOL                | -197.3       | -199.99       | -2.69       |
| 575 | p-tert-OCYTLPHENOL           | -392.44      | -361.24       | 31.2        |
| 576 | p-tert-AMYLPHENOL            | -300.85      | -280.62       | 20.23       |
| 577 | p-CUMYLPHENOL                | -172.25      | -173.53       | -1.28       |
| 578 | 2,4-PENTANEDIOL              | -556.35      | -530.05       | 26.3        |
| 579 | 3-METHYL-trans-2-PENTENE     | -94.56       | -111.09       | -16.53      |
| 580 | 5-METHYL-1-HEXENE            | -100         | -137.96       | -37.96      |
| 581 | DECAN-1,10-DIOL              | -699.71      | -664.42       | 35.29       |
| 582 | 1,4-CYCLOHEXANEDIMETHANOL    | -584.6       | -557.02       | 27.58       |
| 583 | 2-METHYL-1-OCTENE            | -165.1       | -191.71       | -26.61      |
| 584 | 2-METHYL-1-HEPTENE           | -134.18      | -164.84       | -30.66      |
| 585 | TRIMELLITIC ACID             | -1179.2      | -1046.4       | 132.8       |
| 586 | TRILACTIC ACID               | -1547        | -1457.08      | 89.92       |
| 587 | LINOLENIC ACID               | -526.43      | -664.83       | -138.4      |
| 588 | AZELAIC ACID                 | -1059.3      | -922.44       | 136.86      |
| 589 | NEOPENTANOIC ACID            | -564         | -476.4        | 87.6        |
| 590 | PENTADECANOIC ACID           | -861.7       | -745.15       | 116.55      |
| 591 | 2-ETHYL HEXANOIC ACID        | -635.1       | -557.02       | 78.08       |
| 592 | n-HEPTANOIC ACID             | -611.4       | -530.15       | 81.25       |
| 593 | NEOHEXANOIC ACID             | -595         | -503.27       | 91.73       |
| 594 | NEOHEPTANOIC ACID            | -613.53      | -530.15       | 83.38       |
| 595 | n-HEPTADECANOIC ACID         | -924.4       | -798.9        | 125.5       |
| 596 | NONADECANOIC ACID            | -984         | -852.64       | 131.36      |
| 597 | n-EICOSANIC ACID             | -1011.9      | -879.52       | 132.38      |
| 598 | FUMARIC ACID                 | -812.2       | -734.42       | 77.78       |
| 599 | PIMELIC ACID                 | -1009.8      | -868.69       | 141.11      |
| 600 | SUBERIC ACID                 | -1038        | -895.57       | 142.43      |
| 601 | CINNAMIC ACID                | -336.9       | -315.67       | 21.23       |
| 602 | ACETOXYACETIC ACID           | -879.7       | -788.07       | 91.63       |
| 603 | SEBACIC ACID                 | -1082.6      | -949.31       | 133.29      |
| 604 | ITACONIC ACID                | -841.1       | -761.3        | 79.8        |
| 605 | SUCCINIC ACID                | -940.4       | -788.07       | 152.33      |
| 606 | GLUTARIC ACID                | -959.9       | -814.94       | 144.96      |
| 607 | PYROMELLITIC ACID            | -1570.8      | -1411.82      | 158.98      |
| Compound                        | E2007 | E2008 | E2007 - E2008 | \% Error |
|--------------------------------|-------|-------|---------------|---------|
| IBUPROFEN                      | -559.53 | -476.82 | 82.71         |
| METHYL MALEIC ANHYDRIDE        | -504.55 | -511.56 | -7.01         |
| sec-BUTYL FORMATE              | -482.76 | -476.4  | 6.36          |
| tert-BUTYL FORMATE             | -499.65 | -476.4  | 23.25         |
| n-HEXYL FORMATE                | -518.49 | -530.15 | -11.66        |
| n-HEPTYL FORMATE               | -542.98 | -557.02 | -14.04        |
| CYCLOHEXYL FORMATE             | -495.52 | -476.5  | 19.02         |
| tert-BUTYL ACETATE             | -561.02 | -503.27 | 57.75         |
| METHYL ISOBYTRATE              | -501.76 | -476.4  | 25.36         |
| ETHYL ISOBYTRATE               | -538.74 | -503.27 | 35.47         |
| ISOPROPYL ACRYLATE             | -419.4  | -449.63 | -30.23        |
| BENZYL FORMATE                 | -305.13 | -342.44 | -37.31        |
| CYTET METHACRYLATE             | -742.81 | -825.87 | -83.06        |
| DIMETHYL-2,6-NAPHTHALENEDICARBOXYLATE | -709.5 | -654.47 | 55.03         |
| CYCLOHEXYL ACETATE             | -553.48 | -503.38 | 50.1          |
| n-NONYL n-UNDECYL PHTHALATE    | -1140   | -1218.48 | -78.48        |
| DIMISONONYL PHTHALATE          | -1237   | -1164.73 | 72.27         |
| DIETHYL PHTHALATE              | -776.6  | -788.48 | -11.88        |
| DIMETHYL PHTHALATE             | -677.81 | -734.73 | -56.92        |
| DIETHYL SUCINNATE              | -913.07 | -895.57 | 17.5          |
| DIHEXYL ADIPATE                | -1161.6 | -1164.31 | -2.71         |
| ETHYLIDINE DIACETATE           | -865.97 | -841.82 | 24.15         |
| DIBUTYL MALEATE                | -772.2  | -949.42 | -177.22       |
| METHYL DODECANOATE             | -693    | -691.4  | 1.6           |
| DIETHYL MALEATE                | -798.18 | -841.92 | -34.74        |
| DIMETHYL MALEATE               | -680.85 | -788.17 | -107.32       |
| DIPROPYL MALEATE               | -785.11 | -895.67 | -110.56       |
| sec-BUTYL ACRYLATE             | -436.8  | -476.5  | -39.7         |
| VINYL PIVALATE                 | -429.1  | -476.5  | -47.4         |
| DIMETHYL CARBONATE             | -607.27 | -618.74 | -11.47        |
| n-PROPYL BENZOATE              | -397.7  | -396.19 | 0.52          |
| ETHYL ISOPROPYL ETHER          | -315.8  | -333.95 | -18.15        |
| ETHYL n-HEXYL ETHER            | -381.01 | -414.58 | -33.57        |
| 1,3-DIOXANE                    | -377.5  | -449.52 | -72.02        |
| 1,2-DIETHOXYETHANE             | -451.43 | -556.92 | -105.49       |
| 2,3-DICHLOROPROPENE            | -73.3   | -84.21  | -10.91        |
| n-PENTADECYL BENZENE           | -355.24 | -353.27 | 0.57          |
| n-HEXADECYL BENZENE            | -414.67 | -380.15 | 34.52         |
| n-HEPTADECYL BENZENE           | -442.5  | -342.02 | 25.88         |
| n-OCTADECYL BENZENE            | -469.9  | -433.89 | 36.01         |
| 1,3-DICHLOROHEXAFLUOROPROPA    | -1321.8 | -1347.63 | -25.83        |
| 1,2-DICHLOROHEXAFLUOROCYCLOBUTANE | -1282.7 | -1230.86 | -31.65        |
| 3,3,3-TRIFLUOROPROPENE         | -613.2  | -635.35 | -21.15        |
| 1,1,2-TRIFLUOROETHANE          | -675.9  | -662.12 | 13.78         |
| PERFLUORO-n-HEXADECANE          | -7251   | -7228.88 | -38.88        |
| PERFLUOROMETHYLCYCLOPENTANE    | -2533   | -2530.64 | 2.36          |
| 1,1,1,2,2-PENTAFLUOROPROPA     | -1111   | -1092.26 | 18.74         |
| 1,1,1,2,3,3-HEXAFLUOROPROPA    | -1333   | -1293.89 | 31.11         |
| BENZOTRIFLUORIDE               | -636.7  | -581.91 | 54.79         |
| 2-BROMOBUTANE                  | -155.1  | -137.86 | 17.24         |
| BROMOCHLOROMETHANE             | -76.01  | -84.11  | -8.1          |
| HALOTHANE                      | -720    | -715.87 | 4.13          |
| 1,2-DIFLUOROETHANE             | -447.7  | -460.49 | -12.79        |
| PENTACHLOROFLUOROETHANE        | -382    | -393.24 | -28.94        |
| 1,2-DICHLORO-1,1,2-TRIFLUOROETHANE | -735.55 | -715.87 | 19.68         |
| 2-CHLORO-1,1,2-TETRAFLUOROETHANE | -924.7  | -890.63 | 34.07         |
| 1,1-DICHLORO-1-FLUROETHANE     | -366.4  | -312.61 | 16.49         |
| 1,1,1,2-TETRAFLUOROETHANE      | -895.79 | -863.75 | 32.04         |
| HEXAFLUOROACETONE              | -1460   | -1436.33 | 18.27         |
| OCTAFLUOROETHANE               | -1783.2 | -1697.14 | 46.86         |
| OCTAFLUOROPROPA                | -1648   | -1670.37 | -22.37        |
| OCTAFLUOROCYCLOBUTANE          | -1528   | -1670.37 | -142.37       |
| 1,1,1-TRICHLOROFUOROETHANE     | -337.1  | -339.49 | -2.39         |
| Chemical Name                        | V(T)   | V(S)   | V(L)   |
|-------------------------------------|--------|--------|--------|
| 1,1,2,2-TETRAFLUOROETHANE          | -892.4 | -863.75| 28.65  |
| p-BROMOTOLUENE                     | 17.14  | -3.9   | -21.04 |
| n-HEXYL IODIDE                     | -146.4 | -191.61| -45.21 |
| BROMOTRIFLUOROMETHANE              | -648.98| -662.12| -13.14 |
| DIBROMODIFLUOROMETHANE             | -386.6 | -487.37| -100.77|
| CHLOROTRIFLUOROETHYLENE            | -555.3 | -635.35| -80.05 |
| HEXAFLUOROETHANE                   | -1343.9| -1267.01| 76.89  |
| 1-CHLORO-1,1-DIFLUOROETHANE        | -329.7 | -487.37| 42.33  |
| n-HEXYLAMINE                       | -177.12| -191.61| -14.49 |
| n-HEPTYLAMINE                      | -201.33| -218.48| -17.15 |
| n-OCTYLAMINE                       | -226.02| -245.36| -19.34 |
| n-NONYLAMINE                       | -250.44| -272.23| -21.79 |
| n-DECYLAMINE                       | -275.19| -299.11| -23.92 |
| n-DODECYLAMINE                     | -368.18| -352.86| 15.32  |
| CYCLOHEXYL ISOCYANATE              | -200.64| -253.64| -53    |
| N,N'-DI-tert-BUTYLETHYLENEDIAMINE   | -264.9 | -325.98| -61.08 |
| DICYCLOHEXYLAMINE                  | -246.4 | -245.56| 0.84   |
| N-METHYLCYCLOHEXYLAMINE            | -149.52| -164.84| -15.32 |
| N-Aminoethyl ETHANOLAMINE          | -280.19| -360.83| -80.6  |
| PHENYL ISOCYANATE                  | -61.08 | -92.7  | -31.62 |
| ISOQUINOLINE                       | 134.2  | 130.11 | -4.09  |
| p-AMINODIPHENYL                    | 81     | 76.31  | -4.69  |
| 2,6-DIETHYLANILINE                | -84.23 | -84.52 | 0.29   |
| 3-METHYLPYRIDINE                   | 61.9   | 22.97  | -38.93 |
| 4-METHYLPYRIDINE                   | 59.2   | 22.97  | -36.23 |
| ETHYL 1-BUTYL SULFIDE              | -187.3 | -191.61| -4.31  |
| tert-NONYL MERCAPTAN               | -266.22| -272.23| -6.01  |
| 2-METHYLTETRAHYDROPHENETE          | 44.6   | 23.03  | -21.57 |
| 3-METHYLTETRAHYDROPHENETE          | 43.1   | 23.03  | -20.07 |
| CAMPHOR                            | -319.4 | -307.39| 12.01  |
| N-METHYLFORMAMIDE                  | -241.48| -226.56| 14.92  |
| DIACETONE ALCOHOL                  | -592.79| -503.27| 89.52  |
| FURFURYL ALCOHOL                   | -276.2 | -342.29| -66.09 |
| N,N-DIMETHYLACETAMIDE              | -278.3 | -280.31| -2.01  |
| ACETAMINOPHEN                      | -396.04| -369.32| 26.72  |
| p-METHOXYPHENOL                    | -335.51| -369.21| -33.7  |
| 2-METHOXYETHANOL                   | -416.32| -476.3 | -59.98 |
| 2-ETHOXYETHANOL                    | -448.22| -503.17| -54.95 |
| 2-BUTOXYETHANOL                    | -497.4 | -556.92| -59.52 |
| 2-(2-METHOXYETHOXY)ETHANOL         | -589.99| -726.14| -136.15|
| 2-(2-ETHOXYETHOXY)ETHANOL          | -626.28| -753.01| -126.73|
| 2-Aminoethoxyethanol               | -438.05| -530.05| 92.04  |
| ETHYL CHLOROACETATE                | -509.3 | -476.4 | -31.9  |
| 2-(2-METHOXYETHOXY)ETHOXYETHANOL   | -786.4 | -975.98| -189.58|
| SUCCINIMIDE                        | -460.25| -369.11| 91.14  |
| 4-CARBOXYBENZALDEHYDE              | -544.91| -484.89| 60.02  |
| THIOGLYCOLIC ACID                  | -454.56| -422.65| 31.91  |
| 2-HYDROXYETHYL METHACRYLATE        | -576.15| -645.72| -69.57 |
| METHYL LACTATE                     | -643.1 | -645.62| -2.52  |
| 2-METHOXY PROPANOL-1               | -449.47| -503.17| -53.7  |
| alpha-METHYLBenzyL ALCOHOL FORMATE | -347.1 | -369.32| -22.22 |
| 2-FORMYL BENZOIC ACID              | -531.54| -484.89| 46.65  |
| 2-HYDROXYACETOPHENONE              | -342.2 | -342.44| -0.24  |
| 4-HYDROXYACETOPHENONE              | -364.3 | -342.44| 21.86  |
| 4-HYDROXYSTYRENE                   | -109.67| -146.35| -36.68 |
| ACETYL SALICYLIC ACID              | -815.6 | -707.86| 107.74 |
| p-PHENETIDINE                      | -172.6 | -226.87| -54.27 |
| ACETOL                             | -414.15| -422.65| -8.5   |
| o-CHLOROPHENOL                     | -172.35| -173.12| -0.77  |
| 1-ISOPROPOXY-2-PROPANOL            | -529.6 | -556.92| -27.32 |
| ISOPHTHALOYL CHLORIDE              | -367.5 | -342.55| 24.95  |
| 4-FORMYL MorPHOLINE                | -369.9 | -449.63| -79.73 |
| FLUOSULFONIC ACID                  | -795.78| -712.98| 82.8   |
| No. | Compound                                      | Δν (cm⁻¹) | Δδ (ppm) | J (Hz) |
|-----|-----------------------------------------------|-----------|----------|--------|
| 734 | CHLOROSULFONIC ACID                           | -651.14   | -538.22  | 112.92 |
| 735 | FERRIC OXIDE                                  | -825.5    | -1071.38 | -245.88|
| 736 | ZINC SULFATE                                  | -980.14   | -947.25  | 32.89  |
| 737 | 3-ETHYL HEPTANAL                              | -369.5    | -387.8   | -18.3  |
| 738 | DIAMYL KETONE                                 | -446.5    | -441.55  | 4.95   |
| 739 | 2-BUTYL-1-DECANOL                             | -567.6    | -575.82  | 8.2    |
| 740 | 2-METHYL-1-TRIDECANOL                         | -566.9    | -575.82  | -9.92  |
| 741 | 2-METHYL-DODECAN-1-OL                         | -552.6    | -548.95  | 3.65   |
| 742 | 4-METHYL-1-OCTANOL                            | -462.6    | -441.45  | 21.15  |
| 743 | 3-ETHYL-1-HEPTANOL                            | -440.7    | -441.45  | -0.75  |
| 744 | THYMOL                                        | -277.9    | -253.74  | 24.16  |
| 745 | 1-METHYL-3-HYDROXY-5-ISOPROPYL BENZENE        | -300      | -253.74  | 46.26  |
| 746 | 1-METHYL-3-HYDROXY-6-ISOPROPYL BENZENE        | -295      | -253.74  | 41.26  |
| 747 | trans-1,8-TERPIN                              | -706.9    | -610.77  | 96.13  |
| 748 | 7-METHYL-1-OCTENE                             | -154.5    | -191.71  | 37.21  |
| 749 | 2-METHYL-1-NONEINE                            | -188.7    | -218.59  | 29.89  |
| 750 | 8-METHYL-1-NONEINE                            | -180.2    | -218.59  | 38.39  |
| 751 | trans-2-DECENE                                | -187.1    | -218.59  | 31.49  |
| 752 | cis-2-DODECENE                                | -233.7    | -272.34  | 38.64  |
| 753 | trans-2-DODECENE                              | -239      | -272.34  | 33.34  |
| 754 | CYCLOPROPANE CARBOXYLIC ACID                  | -396.5    | -395.88  | 0.62   |
| 755 | MALONIC ACID                                  | -891      | -761.19  | 129.81 |
| 756 | n-PROPYL ACETATE                              | -410.1    | -449.63  | 39.53  |
| 757 | sec-BUTYL ACETATE                             | -409      | -449.63  | 40.63  |
| 758 | VINYLETHYLENE CARBONATE                      | -555.4    | -565.2   | -9.8   |
| 759 | DIOCYL ADIPATE                                | -1266     | -1271.81 | 5.81   |
| 760 | DI(2-ETHYLHEXYL)ADIPATE                      | -1265.3   | -1271.81 | 6.51   |
| 761 | DODECYL BROMIDE                               | -344.7    | -352.86  | -8.16  |
| 762 | 1,2-DIBROMODODECANE                           | -367.8    | -379.73  | 11.93  |
| 763 | TRIFLUORORIODOMETHANE                        | -589.1    | -662.12  | 73.02  |
| 764 | DIFLUOROMETHYL TRIFLUOROMETHYL ETHER          | -1316     | -1261.47 | 54.53  |
| 765 | CYCLOPROPANE CARBOXYLIC ACID                  | -190.5    | -226.66  | 36.16  |
| 766 | 6-AMINOHEXANAMIDE                             | -400.7    | -360.93  | 39.77  |
| 767 | HEXANAMIDE                                    | -423.1    | -334.06  | 89.04  |
| 768 | TRI-n-OCTYLAMINE                              | -585.01   | -675.35  | 90.34  |
| 769 | DIAMYLAMINE                                   | -262.21   | -299.11  | -36.9  |
| 770 | TRIAMYLAMINE                                  | -366.82   | -433.48  | 66.66  |
| 771 | UNDECYLAMINE                                  | -299.52   | -325.98  | 26.46  |
| 772 | NIAIN                                         | -349.8    | -315.57  | 29.33  |
| 773 | L-PHENYLALANINE                               | -466.9    | -396.19  | 70.71  |
| 774 | DI-2-ETHYLHEXYLAMINE                          | -415.9    | -460.35  | 44.45  |
| 775 | BENZIDINE                                     | 70.7      | 49.43    | 21.27  |
| 776 | DICYANDIAMIDE                                 | 24.9      | -3.8     | 28.7   |
| 777 | DI-tert-BUTYL DISULFIDE                       | -253      | -272.23  | 19.23  |
| 778 | DI-tert-BUTYL SULFIDE                         | -232.3    | -245.36  | 13.06  |
| 779 | 2-METHYLCYCLOPENTANE                          | -105      | -111.09  | 6.09   |
| 780 | METHYL ISOPROPYL SULFIDE                      | -123.5    | -137.86  | 14.36  |
| 781 | 2-ETHYLPHENOL                                 | 16.61     | -3.85    | 20.46  |
| 782 | 2-n-PROPYLPHENOL                              | -8.96     | -30.72   | 21.76  |
| 783 | ETHYL PROPYL DISULFIDE                        | -146.2    | -191.61  | 45.41  |
| 784 | DIISOPENTYL SULFIDE                           | -282      | -299.11  | 17.11  |
| 785 | ETHYLENE GLYCOL 2-ETHYLHEXYL ETHER            | -597.87   | -637.54  | 39.67  |
| 786 | PROPYLENE GLYCOL ETHYL ETHER ACETATE          | -608.2    | -726.24  | 118.04 |
| 787 | DIPROPYLENE GLYCOL t-BUTYL ETHER              | -801.39   | -860.51  | 59.12  |
| 788 | DICHLOROACETIC ACID                           | -496.3    | -449.52  | 46.78  |
| 789 | PROPYLENE GLYCOL MONOMETHYL ETHER             | -447.74   | -503.17  | 55.43  |
| 790 | PROPYLENE GLYCOL MONOMETHYL ETHER             | -660.85   | -779.89  | 119.04 |
| 791 | PROPYLENE GLYCOL 1-tert-BUTYL ETHER           | -610.36   | -583.79  | 26.57  |
| 792 | TRIPROPYLENE GLYCOL MONOMETHYL ETHER          | -884.09   | -1056.61 | 172.52 |
| 793 | DIETHYLENE GLYCOL MONOPROPYL ETHER            | -647.93   | -779.89  | 131.96 |
| 794 | 2-(2-ETHOXYETHOXY)ETHOXYETHANOL               | -844.47   | -1056.61 | 212.14 |
| 795 | 2-(2-ETHOXYETHOXY)ETHOXYETHANOL               | -796.01   | -1002.86 | 206.85 |
| 796 | 2-HEXOXYETHANOL                               | -560.3    | -610.67  | 50.37  |
| No. | Chemical Name                        | Log P | Kow  | Log P | Kow  |
|-----|------------------------------------|-------|------|-------|------|
| 797 | MONOOLEIN                         | -1175 | -1244.94 | -69.94 |
| 798 | PROPYLENE GLYCOL, n-PROPYL Ether   | -506  | -556.92  | -50.92 |
| 799 | DIETHYLENE GLYCOL MONOBUTYL Ether Acetate | -883.71 | -1002.96 | -119.25 |
| 800 | 3-HYDROXY-2-METHYL PROPIONALDEHYDE | -427.87 | -476.4  | -48.53 |
| 801 | HYDROXYACETONITRILE               | -141.77 | -172.91  | -31.14 |
| 802 | DIOLEIN                           | -1670  | -1817.48  | -147.48 |
| 803 | TRIOLEIN                          | -2161  | -2390.03  | -229.03 |
| 804 | sec-BUTENYL GLYCOL ETHER          | -385.3 | -503.27  | -117.97 |
| 805 | SUCROSE                           | -2226.1 | -2375.72  | -149.62 |
| 806 | PENTAFLUOROETHYL TRIFLUOROVINYL ETHER | -1900 | -1866.47  | 33.53 |
| 807 | TRIFLUOROMETHYL TRIFLUOROVINYL ETHER | -1521 | -1463.1  | 57.9 |
| 808 | DIPROPYLENE GLYCOL MONOOETHYL ETHER | -721.6 | -806.76  | -85.16 |
| 809 | TRIPROPYLENE GLYCOL MONOOETHYL ETHER | -957.4 | -1083.48 | -126.08 |
| 810 | 1-ETHOXY-2-PROPANOL               | -492.7 | -530.05  | 37.35 |
| 811 | 1-tert-BUTOXY-2-[2-(HYDROXY)PROPOXY]PROPANE | -774.9 | -860.51  | 85.61 |
| 812 | METHYL GLYCOLATE                  | -609.4 | -618.74  | -9.34 |
| 813 | tert-BUTYL METHACRYLATE           | -498.2 | -557.02  | -58.82 |
| 814 | gamma-AMINOPROPYLTRIETHOXYSILANE  | -1022  | -1153.96 | -131.96 |
| 815 | (3-METHYLACRYLOXYPROPYL)TRICHLOROSILANE | -921  | -850.58  | 70.42 |
| 816 | METHYL DICHLOROSILANE             | -435.5 | -377.56  | 59.99 |
| 817 | FERROUS CHLORIDE                  | -341.83 | -350.69  | -8.86 |
| 818 | FERRIC CHLORIDE                   | -399.41 | -377.56  | 21.85 |
| 819 | DIMETHYLCHELOROSILANE             | -326.35 | -377.56  | -51.21 |
| 820 | TRIMETHYLCHELOROSILANE            | -382.61 | -404.43  | -21.82 |
| 821 | DIMETHYLCHLOROSILANE              | -480.4 | -404.43  | 75.97 |
| 822 | DIPHENYLCHLOROSILANE              | -238   | -244.02  | -6.02 |
| 823 | DICHLORODIETHYLISILANE            | -530.7 | -458.18  | 72.52 |
| 824 | ACETOVANILLONE                    | -529.56 | -565.41  | -35.85 |
| 825 | VANILLIN                          | -453.4 | -538.54  | -85.14 |
| 826 | DIGLYCOLIC ACID                   | -1080.4 | -984.16  | 96.24 |
| 827 | LEVULINIC ACID                    | -697.05 | -618.85  | 78.2 |
| 828 | MALIC ACID                        | -1105.4 | -984.16  | 121.24 |
| 829 | GUAIACOL                          | -325.78 | -369.21  | -43.43 |
| 830 | ETHYLENE GLYCOL, MONOPROPYL ETHER | -473.09 | -530.05  | -56.96 |
| 831 | 2-(2-BUTOXYETHOXY)ETHANOL         | -674.4 | -806.76  | 132.36 |
| 832 | ETHYLENEDIAMINETETRAACETIC ACID   | -1759.5 | -1680.15 | 79.35 |
| 833 | TRICHLOROACETALDEHYDE             | -234.5 | -280.31  | -45.81 |
| 834 | TRICHLOROACETIC ACID              | -503.3 | -476.4  | 26.9 |
| 835 | CHLOROACETALDEHYDE                | -252.69 | -226.56  | 26.13 |
| 836 | DICHLOROACETALDEHYDE              | -218.07 | -253.43  | -35.36 |
| 837 | ETHYL CHLOROFORMATE               | -505.2 | -440.52  | 55.68 |
| 838 | METHOXYACETIC ACID                | -627.04 | -618.74  | 8.3 |
| 839 | METHYL CHLOROFORMATE              | -460.74 | -422.65  | 38.09 |
| 840 | DEXTROSE                          | -1273.3 | -1287.65 | 14.35 |
| 841 | VINYLTRIMETHOXYLSILANE            | -835.9 | -965.94  | 130.04 |
| 842 | TRIMETHOXYLSILANE                 | -833   | -965.84  | 132.84 |
| 843 | TRIMETHYL SILANOL                 | -545.2 | -573.65  | 28.45 |
| 844 | ETHYL ALUMINUM SESQUICHLORIDE     | -970.6 | -832.26  | 138.34 |
| 845 | SULFAMIC ACID                     | -674.88 | -538.22  | 136.66 |
| 846 | BIS(CHLOROMETHYL)ETHER            | -280.58 | -307.08  | -26.5 |
| 847 | 3-AMINO-1-PROPANOL                | -291.34 | -307.08  | -15.74 |
| 848 | 1-AMINO-2-PROPANOL                | -294.1 | -307.08  | -12.98 |
| 849 | ETHYL THIOLACETATE                | -231.1 | -280.31  | -49.21 |
| 850 | ACETOACETANILIDE                  | -403.33 | -369.42  | 33.91 |
| 851 | LYSINE                            | -678.69 | -557.02  | 121.67 |
| 852 | DIMETHYL SULFATE                  | -735.5 | -761.19  | -25.69 |
| 853 | DIETHYL SULFATE                   | -813.2 | -814.94  | -1.74 |
| 854 | L-GLUTAMIC ACID                   | -1009.7 | -841.82  | 167.88 |
| 855 | ASCORBIC ACID                     | -1164.6 | -1180.36 | 15.76 |
| 856 | 6-HYDROXYHEXANOIC ACID            | -779.32 | -699.37  | 79.95 |
| 857 | CITRIC ACID                       | -1543.8 | -1376.45 | 167.35 |
| 858 | LACTIC ACID                       | -682.96 | -618.74  | 64.22 |
| 859 | TARTRIC ACID                      | -1289.5 | -1180.25 | 109.25 |
4. Conclusions

In this present study, a simple five descriptors linear model was presented. This model was the result of a QSPR study on the standard enthalpy of formation of 1115 compounds. These compounds have been selected from all families of compounds as a result there are no specific limit in application of this model. Also the simplicity of the use of it is one of the advantages of this model.

All molecular descriptors of this model can be easily calculated from the chemical structure of a molecule.
**Table 4.** The predicted $\Delta H_f$ by the Eq. (2) for test set as an excluded data set.

| ID | Name                                      | $\Delta H_f$ (kJ/mol) | Res   |
|----|--------------------------------------------|------------------------|-------|
|    |                                            | DIPPR 801              | Calculated from Eq. (2) |
| 1  | 2-METHYLPENTANE                           | -204.64                | -164.73 | 39.91  |
| 2  | 2-METHYLBUTANE                            | -229.49                | -191.61 | 37.88  |
| 3  | n-OCTANE                                  | -249.78                | -218.48 | 31.3   |
| 4  | 3-METHYLHEPTANE                           | -252.34                | -218.48 | 33.86  |
| 5  | 2,5-DIMETHYLHEXANE                        | -260.37                | -218.48 | 41.89  |
| 6  | 3,4-DIMETHYLHEXANE                        | -251.83                | -218.48 | 33.35  |
| 7  | 2,2,3,3-TETRAETHYLHEXANE                  | -268.61                | -218.48 | 50.13  |
| 8  | 2,2,5-TRIMETHYLHEXANE                     | -293.3                 | -245.36 | 47.94  |
| 9  | 2,2,3,4-TETRAETHYLHEXANE                  | -277.7                 | -245.36 | 32.34  |
| 10 | 2,3,3,4-TETRAETHYLHEXANE                  | -277.9                 | -245.36 | 32.54  |
| 11 | 2,2,3,3-TETRAETHYLHEXANE                  | -303.47                | -272.23 | 31.24  |
| 12 | n-HEPTADECANE                             | -479.86                | -460.35 | 19.51  |
| 13 | 2,2-DIMETHYLOCTANE                        | -313.12                | -272.23 | 40.89  |
| 14 | n-DECOSANE                                | -623.61                | -540.98 | 82.63  |
| 15 | n-TETRACOSANE                             | -739.31                | -648.48 | 90.83  |
| 16 | 3-METHYLNONANE                            | -303.59                | -272.23 | 31.36  |
| 17 | 4-METHYLNONANE                            | -304.1                 | -272.23 | 31.87  |
| 18 | 2-METHYLOCTANE                            | -280.6                 | -245.36 | 35.24  |
| 19 | ISOPROPYLCYCLOPENTANE                     | -190.09                | -164.84 | 25.25  |
| 20 | n-BUTYLCYCLOPENTANE                       | -214.2                 | -191.71 | 22.49  |
| 21 | n-BUTYLCYCLOHEXANE                        | -263.09                | -218.59 | 44.5   |
| 22 | BICYCLOHEXYL                              | -273.7                 | -218.69 | 55.01  |
| 23 | cis-2-PENTENE                             | -53.49                 | -84.21  | -30.72 |
| 24 | trans-2-PENTENE                           | -57.98                 | -84.21  | -26.23 |
| 25 | 2-METHYL-2-BUTENE                         | -68.07                 | -84.21  | -16.14 |
| 26 | trans-3-HEXENE                            | -86.06                 | -111.09 | -25.03 |
| 27 | 3-METHYL-cis-2-PENTENE                    | -94.47                 | -111.09 | -16.62 |
| 28 | 2,3-DIMETHYL-2-BUTENE                     | -102.42                | -111.09 | -8.67  |
| 29 | 4-METHYL-1-HEPTENE                        | -126.1                 | -164.84 | -38.74 |
| 30 | trans-2-OCTENE                            | -135                   | -164.84 | -29.84 |
| 31 | 2,4,4-TRIMETHYL-2-PENTENE                 | -142.42                | -164.84 | -22.42 |
| 32 | 1-DECENE                                  | -172.3                 | -218.59 | -46.29 |
| 33 | 1-PENTADECENE                             | -301.12                | -352.96 | -51.84 |
| 34 | 1-HEPTADECENE                             | -349.83                | -406.71 | -56.88 |
| 35 | 1-NONADECENE                              | -399.59                | -460.46 | -60.87 |
| 36 | p-tert-BUTYL ETHYLBENZENE                 | -131.46                | -111.4  | 20.06  |
| 37 | m-DIISOPROPYLBENZENE                      | -132.4                 | -111.4  | 21     |
| 38 | 1,2,4-TRIETHYLBENZENE                     | -134.05                | -111.4  | 22.65  |
| 39 | HEXAETHYLBENZENE                          | -329.6                 | -272.65 | 56.95  |
| 40 | p-TERPHENYL                               | 150.25                 | 156.52  | 6.27   |
| 41 | TRIPHENYLMETHANE                          | 171.2                  | 129.64  | -41.56 |

**Note:** Table entries are calculated from Eq. (2) and compared with DIPPR 801 values.
|   | Compound          | m/z  | n/z  | epsilon  |
|---|-------------------|------|------|----------|
| 42 | 2-METHYLINDENE    | 60.78| 49.64| -11.14   |
| 43 | INDENE            | 110.42| 76.52| -33.9    |
| 44 | PENTANAL          | -267.3| -280.31| -13.01  |
| 45 | 3-METHYLHEXANAL   | -315.39| -334.06| -18.67  |
| 46 | TRIDECANAL        | -470.62| -495.3| -24.68   |
| 47 | GLYCOL ALDEHYDE   | -404.2| -395.78| 8.42     |
| 48 | METHACROLEIN      | -145.04| -199.79| -54.75   |
| 49 | p-TOLUALDEHYDE    | -120.56| -146.35| -25.79   |
| 50 | BENZALDEHYDE      | -86.82| -119.47| -32.65   |
| 51 | SALICYLALDEHYDE   | -265.7| -315.57| -49.87   |
| 52 | m-TOLUALDEHYDE    | -123.4| -146.35| -22.95   |
| 53 | PARALDEHYDE       | -673.2| -699.37| -26.17   |
| 54 | ACETONE           | -248.1| -226.56| 21.54    |
| 55 | 3-PENTANONE       | -296.51| -280.31| 16.2     |
| 56 | 5-HEXEN-2-ONE     | -197.4| -253.54| -56.14   |
| 57 | 2-PENTANONE       | -297.29| -280.31| 16.98    |
| 58 | METHYL ISOPROPYL KETONE | -299.5 | -280.31| 19.19    |
| 59 | 2-HEPTANONE       | -348.2| -334.06| 14.14    |
| 60 | 5-METHYL-2-HEXANONE | -350.93| -334.06| 16.87    |
| 61 | ISOPHORONE        | -301.4| -280.51| 20.89    |
| 62 | gamma-BUTYROLACTONE | -420.9| -395.88| 25.02    |
| 63 | epsilon-CAPROLACTONE | -477.36| -449.63| 27.73    |
| 64 | gamma-VALEROLACTONE | -461.3| -422.75| 38.55    |
| 65 | ETHYL ISOPROPYL KETONE | -325.9| -307.18| 18.72    |
| 66 | METHYL ISOPROPENYL KETONE | -216.79| -226.66| -9.87    |
| 67 | 2-METHYL-1-PROANOL | -334.7| -307.08| 27.62    |
| 68 | 2-METHYL-2-BUTANOL | -379.5| -333.95| 45.55    |
| 69 | 2-METHYL-1-PENTANOL | -385.8| -360.83| 22.97    |
| 70 | 3-METHYL-3-PENTANOL | -404.93| -360.83| 44.1     |
| 71 | 3-METHYL-2-BUTANOL | -366.64| -333.95| 32.69    |
| 72 | 2-HEPTANOL        | -410.72| -387.7| 23.02    |
| 73 | 5-METHYL-1-HEXANOL | -404.31| -387.7| 16.61    |
| 74 | 4-METHYL-2-PENTANOL | -394.7| -360.83| 33.87    |
| 75 | 1-OCTANOL         | -426.5| -414.58| 11.92    |
| 76 | 2-OCTANOL         | -442.92| -414.58| 28.34    |
| 77 | 2-NONANOL         | -467.91| -441.45| 26.46    |
| 78 | 1-HEXADECANOL     | -686.3| -629.57| 56.73    |
| 79 | 1-OCTADECANOL     | -750| -683.32| 66.68    |
| 80 | 1-EICOSANOL       | -827| -737.07| 89.93    |
| 81 | 1-NONADECANOL     | -785.33| -710.2| 75.13    |
| 82 | CYCLOHEXANOL      | -348.6| -307.18| 41.42    |
| 83 | trans-2-METHYLCHLOROCYANOXANOL | -416.1 | -334.06| 82.04    |
| 84 | L-MENTHOL         | -479.43| -414.68| 64.75    |
| 85 | beta-TERPINEOL    | -369.2| -361.03| 8.17     |
| 86 | 2-METHYL-1-UNDECANOL | -514.5| -522.07| -7.57    |
| 87 | ALLYL ALCOHOL     | -171.1| -226.56| -55.46   |
| 88 | 2,4-XYLENOL       | -228.78| -199.99| 28.79    |
| Molecule                              | DFT Energy (eV) | Experimental Energy (eV) | Error (eV) |
|---------------------------------------|----------------|--------------------------|------------|
| p-CRESOL                              | -199.28        | -173.12                  | 26.16      |
| TRIETHYLENE GLYCOL                    | -804.2         | -949.11                  | -144.91    |
| NEOPENTYL GLYCOL                      | -551.2         | -530.05                  | 21.15      |
| TRIPROPYLENE GLYCOL                   | -921.41        | -1029.73                 | -108.32    |
| 1,2,3-BUTANETRIOL                     | -764.1         | -699.26                  | 64.84      |
| 1,2,4-BUTANETRIOL                     | -745.1         | -699.26                  | 45.84      |
| 1,4-BUTANEDIOL                        | -503.3         | -503.17                  | 0.13       |
| INOSITOL                              | -1362.1        | -1287.65                 | 74.45      |
| 2-METHYLBUTYRIC ACID                  | -554.5         | -476.4                   | 78.1       |
| n-TRADECANOIC ACID                    | -806.6         | -691.4                   | 115.2      |
| n-TETRADECANOIC ACID                  | -833.5         | -718.27                  | 115.23     |
| cis-CROTONIC ACID                     | -347.27        | -395.88                  | -48.61     |
| 2-METHYLOCTANOIC ACID                 | -661.6         | -583.9                   | 77.7       |
| METHACRYLIC ACID                      | -408.09        | -395.88                  | 12.21      |
| BENZOIC ACID                          | -385.2         | -315.57                  | 69.63      |
| o-TOLUIC ACID                         | -416.5         | -342.44                  | 74.06      |
| PHTHALIC ACID                         | -782.07        | -680.98                  | 101.09     |
| ISOPHTHALIC ACID                      | -803           | -680.98                  | 122.02     |
| ETHYL FORMATE                         | -420.5         | -422.65                  | -2.15      |
| METHYL ACETATE                        | -445.8         | -422.65                  | 23.15      |
| n-PROPYL n-BUTYRATE                   | -554.1         | -530.15                  | 23.95      |
| METHYL n-BUTYRATE                     | -490           | -476.4                   | 13.6       |
| n-BUTYL ACRYLATE                      | -433.45        | -476.5                   | -43.05     |
| BENZYL BENZOATE                       | -273.1         | -289.11                  | -16.01     |
| ETHYLENE CARBONATE                    | -586.3         | -565.1                   | 21.2       |
| n-NONYL ACETATE                       | -654.12        | -637.65                  | 16.47      |
| 2-ETHYLHEXYL ACRYLATE                 | -526.06        | -584                     | -57.94     |
| ETHYLENE GLYCOL DICETATE              | -865.43        | -841.82                  | 23.61      |
| ISOBUTYL METHACRYLATE                 | -465.16        | -503.38                  | -38.22     |
| METHYL DECANOATE                      | -640.5         | -637.65                  | 2.85       |
| DIMETHYL-1,4-CYCLOHEXANE DICARBOXYLATE| -948.9         | -895.67                  | 53.23      |
| METHYL ISOPROPYL Ether                | -278.7         | -307.08                  | -28.38     |
| METHYL tert-PENTYL ETHER              | -339.86        | -360.83                  | -20.97     |
| ISOPROPYL ISOBUTYL ETHER              | -370.63        | -387.7                   | -17.07     |
| DIETHYLENE GLYCOL DIETHYL ETHER       | -638.4         | -806.76                  | -168.36    |
| 2,3,4,5,2',3',4',5'-OCTAHYDRO-BIFURYL-(3,3') | -390.5       | -503.38                  | -112.88    |
| CARBON TETRACHLORIDE                  | -128.41        | -137.86                  | -9.45      |
| 3-CHLOROPROPENE                       | -30.8          | -57.34                   | -26.54     |
| 1,4-DICHLORO-cis-2-BUTENE             | -105.65        | -111.09                  | -5.44      |
| m-CHLOROBENZOYL CHLORIDE              | -189.7         | -173.22                  | 16.48      |
| 1,3-DICHLORO-trans-2-BUTENE           | -122.25        | -111.09                  | 11.16      |
| CHLOROFLUOROMETHANE                   | -264           | -258.86                  | 5.14       |
| CHLORODIFLUOROMETHANE                 | -481.6         | -460.49                  | 21.11      |
| 2-CHLORO-1,1-DIFLUOROEThYLENE         | -329           | -433.72                  | -104.72    |
| PERFLUORO-n-OCTANE                    | -3860          | -3847.81                 | 12.19      |
| METHYL BROMIDE                        | -37.7          | -57.23                   | -19.53     |
| PENTAFLUOROETHANE                     | -1100.4        | -1065.38                 | 35.02      |
| 136 | BROMOBENZENE | 60.7 | 22.97 | -37.73 |
| 137 | 1,1-DICHLOROTETRAFLUOROETHANE | -926.8 | -917.5 | 9.3 |
| 138 | DICHLOROFUOROMETHANE | -283.3 | -285.74 | -2.44 |
| 139 | 1-BROMONAPHTHALENE | 116.39 | 103.23 | -13.16 |
| 140 | n-BUTYLAMINE | -127.7 | -137.86 | -10.16 |
| 141 | ISOPROPYLAMINE | -112.3 | -110.98 | 1.32 |
| 142 | n-TETRADECYLAMINE | -424.7 | -406.6 | 18.1 |
| 143 | MONOETHANOLAMINE | -274.47 | -280.2 | -5.73 |
| 144 | HEXANENITRILE | -57.29 | -84.32 | -27.03 |
| 145 | ETHYL MERCAPTAN | -73.6 | -84.11 | -10.51 |
| 146 | n-PROPYL MERCAPTAN | -99.9 | -110.98 | -11.08 |
| 147 | ISOPROPYL MERCAPTAN | -105.9 | -110.98 | -5.08 |
| 148 | METHYL 1-PENTYL SULFIDE | -179.99 | -191.61 | -11.62 |
| 149 | DIETHYL SULFIDE | -119.4 | -137.86 | -18.46 |
| 150 | DI-n-PROPYL DISULFIDE | -171.5 | -218.48 | -46.98 |
| 151 | PHENYL MERCAPTAN | 63.7 | 22.97 | -40.73 |
| 152 | SULFOLANE | -441.64 | -369.11 | 72.53 |
| 153 | CARBONYL FLUORIDE | -638.9 | -576.07 | 62.83 |
| 154 | DICHLOROACETYL CHLORIDE | -280.4 | -280.31 | 0.09 |
| 155 | CHLOROMETHYL METHYL ETHER | -236 | -280.2 | -44.2 |
| 156 | 6-AMINOHEXANOL | -400 | -387.7 | 12.3 |
| 157 | 3-MERCAPTOPROPIONIC ACID | -468.36 | -449.52 | 18.84 |
| 158 | o-CHLOROBENZOIC ACID | -404.83 | -342.44 | 62.39 |
| 159 | ACETONE CYANOHYDRIN | -196.28 | -226.66 | -30.38 |
| 160 | DICHLOROSILANE | -320.49 | -350.69 | -30.2 |
| 161 | 3-NONANONE | -397.4 | -387.8 | 9.6 |
| 162 | 3-NONANONE | -398.3 | -387.8 | 10.5 |
| 163 | 2,6,8-TRIMETHYL-4-NONANONE | -490.9 | -468.43 | 22.47 |
| 164 | 2,7-DIMETHYLOCTANE | -311.3 | -272.23 | 39.07 |
| 165 | 1-PHENYL-2-PROPANOL | -220.17 | -226.87 | -6.7 |
| 166 | 2-PHENYL-1-PROPANOL | -223 | -226.87 | -3.87 |
| 167 | p-TOLUALCOHOL | -209.27 | -199.99 | 9.28 |
| 168 | DINONYLPHENOL | -682.28 | -629.99 | 52.29 |
| 169 | CITRACONIC ACID | -824.46 | -761.3 | 63.16 |
| 170 | 2-ETHYL BUTYRIC ACID | -599.99 | -503.27 | 96.72 |
| 171 | PROPYLENE CARBONATE | -613.2 | -591.97 | 21.23 |
| 172 | GLYCERYL TRIACETATE | -1330.8 | -1260.98 | 69.82 |
| 173 | DI-n-BUTYL PHTHALATE | -842.6 | -895.98 | -53.38 |
| 174 | ISOBUTYL ACRYLATE | -438.95 | -476.5 | -37.55 |
| 175 | DISOBUTYL ETHER | -387.92 | -414.58 | -26.66 |
| 176 | ETHYLAL | -450.41 | -530.05 | -79.64 |
| 177 | PERFLUORO-n-PENTANE | -2608 | -2557.41 | 50.59 |
| 178 | PERFLUORO-n-HEPANE | -3338 | -3417.78 | -79.68 |
| 179 | 1,1,2,3,3,3-HEPTAFLUOROPROPAINE | -1552 | -1495.51 | 56.49 |
| 180 | 2,2-DICHLORO-1,1,2-TRIFLUOROETHANE | -728.38 | -715.87 | 12.51 |
| 181 | 1,1,2-TRICHLOROTRIFLUOROETHANE | -805.8 | -742.75 | 63.05 |
| Entry | Compound | ΔfG° | ΔfH° | ΔfS° |
|-------|-----------|------|------|------|
| 183   | Bromochlorodifluoromethane | -431.37 | -487.37 | -56 |
| 184   | Chloropentafluoroethane | -1123 | -1092.26 | 30.74 |
| 185   | Cyclopentylamine | -95.14 | -111.09 | -15.95 |
| 186   | N,N'-Diphenyl-p-phenylenediamine | 169.08 | 102.77 | -66.31 |
| 187   | Isophorone disocyanate | -429 | -503.69 | -74.69 |
| 188   | Methyl n-butyl sulfide | -142.9 | -164.73 | -21.83 |
| 189   | Tert-dodecyl mercaptan | -338.83 | -352.86 | -14.03 |
| 190   | Triacetone alcohol | -690.06 | -779.99 | -89.93 |
| 191   | 4-Hydroxybutyraldehyde | -417.22 | -449.52 | -32.3 |
| 192   | 2,2,4-Trimethyl-1,3-pentanediol monoisobutyrate | -903 | -860.62 | 42.38 |
| 193   | p-Chlorophenol | -197.7 | -173.12 | 24.58 |
| 194   | 2-Chloroethanol | -307.85 | -280.2 | 27.65 |
| 195   | Chromium trioxide | -578.23 | -724.28 | -146.05 |
| 196   | Ferrous sulfate | -928.85 | -947.25 | -18.4 |
| 197   | Zinc oxide | -347.82 | -439.38 | -91.56 |
| 198   | 6-Methyl-1-octanol | -463.5 | -441.45 | 22.05 |
| 199   | cis-1,8-Terpin | -709.6 | -610.77 | 98.83 |
| 200   | cis-2-Decene | -182.9 | -218.59 | -35.69 |
| 201   | 2,2,4-Trimethyl-1,3-pentanediol disobutyrate | -1118 | -1110.56 | 7.44 |
| 202   | Dimethyl succinate | -845.1 | -841.82 | 3.28 |
| 203   | Benzene-1,2,4-tricarboxylic acid | -1055 | -1127.02 | -72.02 |
| 204   | Dimethylmalonate | -784.8 | -814.94 | -30.14 |
| 205   | Difluoromethyl methyl ether | -642.8 | -656.59 | -13.79 |
| 206   | Di-n-octylamine | -407.3 | -460.35 | -53.05 |
| 207   | 2-Pentanethiol | -151.6 | -164.73 | -13.13 |
| 208   | Di-n-butyl sulfide | -220.5 | -245.36 | -24.86 |
| 209   | Propylene glycol 2-tert-butyl ether | -573.91 | -583.79 | -9.88 |
| 210   | 2-(2-Hexoxyethoxy)ethanol | -742.7 | -860.51 | -117.81 |
| 211   | Diisopropyl glycol n-propyl ether | -737.7 | -833.64 | -95.94 |
| 212   | Crotyl glycol ether | -386.6 | -503.27 | -116.67 |
| 213   | Diethyl sulfite | -600.43 | -672.49 | -72.06 |
| 214   | Dimethylidimethoxysilane | -715.46 | -796.62 | -81.16 |
| 215   | Pyruvic acid | -581.41 | -565.1 | 16.31 |
| 216   | Methyl chloroacetate | -495.6 | -449.52 | 46.08 |
| 217   | Perfluorobutanoic acid | -1924 | -1860.93 | 63.07 |
| 218   | Tridecafluorohexanoic acid | -3215 | -3151.33 | 63.67 |
| 219   | Tert-butylformamide | -340.98 | -307.18 | 33.8 |
| 220   | Methyleneethanolamine | -254.59 | -307.08 | -52.49 |
| 221   | 2-Hydroxypropyl methacrylate | -629.34 | -530.15 | 99.19 |
| 222   | 2-Hydroxypropyl acrylate | -582.5 | -645.72 | -63.22 |
| 223   | Methoxyacetone | -383.4 | -449.52 | -66.12 |
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References

1. Benson S.W. *Thermochemical Kinetics*; Wiley, New York, 1968.
2. Joback, K.G.; Reid R.C. Estimation of pure-component properties from group contributions. *Chem. Eng. Comm.* 1987, 57, 233.
3. Constantinou L.; Gani R. New group contribution method for estimating properties of pure compound. *AIChE J.* 1994, 40, 1697.
4. Katritzky A.R.; Fara D.C. How chemical structure determines physical, chemical, and technological properties: an overview illustrating the potential of quantitative structure-property relationships for fuels science. *Energy & Fuels* 2005, 19, 922.
5. Taskinen J.; Yliruusi J. Prediction of physicochemical properties based on neural network modeling. *Adv. Drug Delivery Rev.* 2003, 55, 1163.
6. Design Institute for Physical Properties Research (DIPPR), American Institute of Chemical Engineers, Project 801, 2006.
7. Hyperchem Release 7.5 for Windows, Molecular Modeling System, Hypercube, Inc., 2002.
8. Talete srl, Dragon for Widows (Software for Molecular Descriptor Calculation). Version 5.4-2006-http://www.talete.mi.it/.
9. Leardi, R.; Boggia, R.; Terrile M. Genetic algorithms as strategy for feature selection. *J. Chemometrics* 1992, 6, 267.
10. Gharagheizi, F. QSPR analysis for intrinsic viscosity of polymer solutions by means of GA-MLR and RBFNN. *Comput. Mater. Sci.* (In press) doi: 10.1016/j.commatsci.2006.11.010.
11. Gharagheizi, F. QSPR studies for solubility parameter by means of genetic algorithm-based multivariate linear regression and generalized regression neural network. *QSAR Comb. Sci.* (In Press) doi: 10.1002/qsar.200630159.
12. Gharagheizi, F.; Mehrpooya, M.; Vatani, A. Prediction of standad chemical exergy by a three-descriptors QSPR model. *Energ. Convers. Manage.* (In Press) doi:10.1016/j.enconman.2007.04.005.
13. Todeschini R.; Consonni, V.; in Manhold, R.; Kubinyi, H.; Temmerman, H. (Series editors), *Handbook of molecular descriptors, Weinheim*, New York, Wiley-VCH, (2000).

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