

Full Research Paper

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, ΔH_f° 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.

$$\Delta H_{reaction} = \sum_p \Delta H_f - \sum_r \Delta H_f \quad (1)$$

where $\Delta H_{reaction}$, $\sum_p \Delta H_f$, and $\sum_r \Delta H_f$ 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 ΔH_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 ΔH_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 ΔH_f° for any compound.

2. Procedures and Methods

2.1. Data set

Many compilations for ΔH_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 ΔH_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 force 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:

$$\Delta H_f^\circ = 50.1688 - 80.52012nSK + 5364546SCBO - 169.21889SCBO - 174.75477nF - 266.57659nHM \quad (2)$$

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_{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_{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 ΔH_f° for training set are presented in the Table-3. Also, the predicted and DIPPR 801 values of ΔH_f° 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.

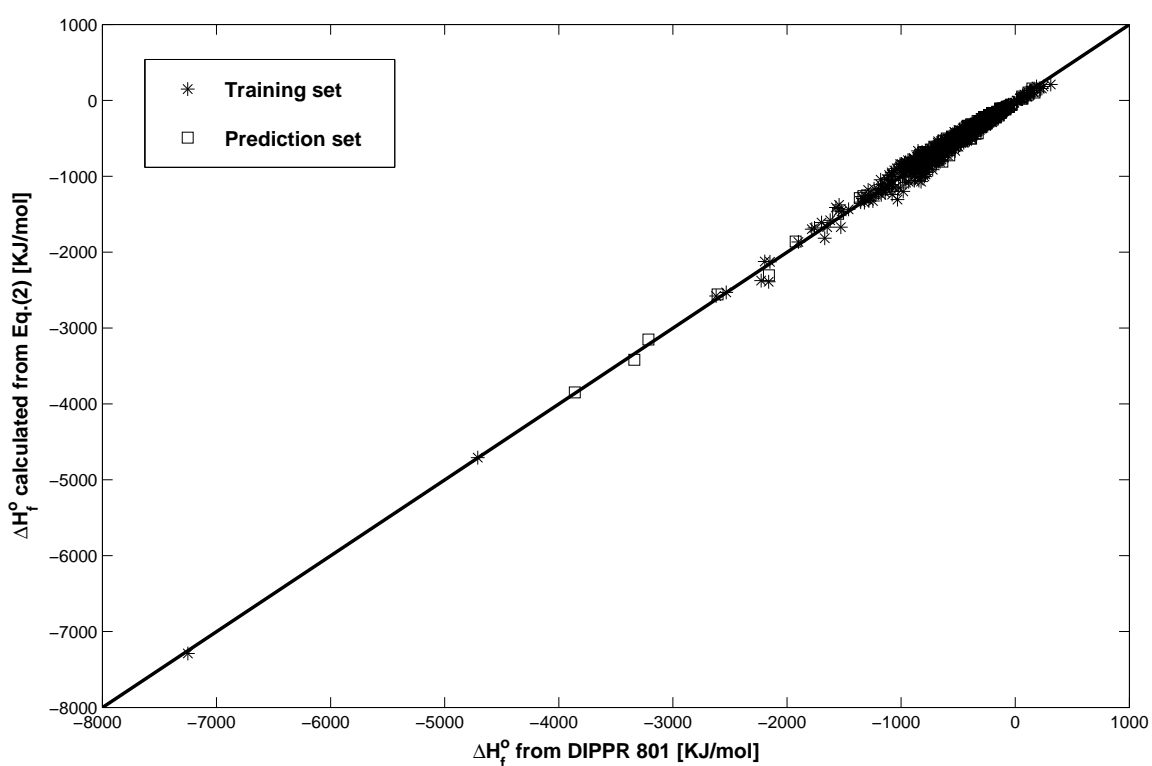


Figure 1. Comparison between the results of Eq. (2) for training set and predicted values for training set.

3. Discussion

In the formation of a molecule from its constituent elements, ΔH_f° , 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 ΔH_f° 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 ΔH_f° .

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

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

ID	Name	ΔH_f° (kJ/mol)		Res
		DIPPR 801	Calculated from Eq. (2)	
1	n-BUTANE	-125.79	-110.98	14.81
2	n-HEXANE	-198.66	-164.73	33.93
3	3-METHYLPENTANE	-202.38	-164.73	37.65
4	n-HEPTANE	-224.05	-191.61	32.44
5	3-METHYLHEXANE	-226.44	-191.61	34.83
6	3-ETHYLPENTANE	-224.56	-191.61	32.95
7	2,2-DIMETHYLPENTANE	-238.28	-191.61	46.67
8	2,3-DIMETHYLPENTANE	-233.09	-191.61	41.48
9	2,4-DIMETHYLPENTANE	-234.6	-191.61	42.99
10	3,3-DIMETHYLPENTANE	-234.18	-191.61	42.57
11	2,2,3-TRIMETHYLBUTANE	-236.52	-191.61	44.91
12	2-METHYLHEPTANE	-255.01	-218.48	36.53
13	4-METHYLHEPTANE	-251.63	-218.48	33.15
14	3-ETHYLHEXANE	-250.41	-218.48	31.93
15	2,2-DIMETHYLHEXANE	-261.88	-218.48	43.4
16	2,3-DIMETHYLHEXANE	-252.59	-218.48	34.11
17	2,4-DIMETHYLHEXANE	-257.02	-218.48	38.54
18	3,3-DIMETHYLHEXANE	-257.53	-218.48	39.05
19	2-METHYL-3-ETHYLPENTANE	-249.58	-218.48	31.1
20	2,2,3-TRIMETHYLPENTANE	-256.9	-218.48	38.42
21	2,2,4-TRIMETHYLPENTANE	-259.16	-218.48	40.68
22	2,3,3-TRIMETHYLPENTANE	-253.51	-218.48	35.03
23	2,3,4-TRIMETHYLPENTANE	-255.01	-218.48	36.53
24	n-NONANE	-274.68	-245.36	29.32
25	3,3,5-TRIMETHYLHEPTANE	-304.76	-272.23	32.53
26	2,4,4-TRIMETHYLHEXANE	-280.2	-245.36	34.84
27	3,3-DIETHYLPENTANE	-275.39	-245.36	30.03
28	2,2,3,3-TETRAMETHYLPENTANE	-278.28	-245.36	32.92
29	2,2,4,4-TETRAMETHYLPENTANE	-279.99	-245.36	34.63
30	SQUALANE	-806.3	-809.72	-3.42
31	n-DECANE	-300.62	-272.23	28.39
32	2,2,5,5-TETRAMETHYLHEXANE	-323.51	-272.23	51.28
33	n-UNDECANE	-326.6	-299.11	27.49
34	n-DODECANE	-352.13	-325.98	26.15
35	n-TRIDECANE	-377.69	-352.86	24.83
36	n-TETRADECANE	-403.25	-379.73	23.52
37	n-PENTADECANE	-428.82	-406.6	22.22
38	n-HEXADECANE	-456.14	-433.48	22.66
39	n-OCTADECANE	-567.14	-487.23	79.91
40	n-NONADECANE	-596.21	-514.1	82.11
41	n-HENEICOSANE	-653.45	-567.85	85.6
42	n-DOCOSANE	-682.07	-594.73	87.34
43	n-TRICOSANE	-710.69	-621.6	89.09

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	2,2,4,4,6,8,8-HEPTAMETHYLNONANE	-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-ETHYLHEPTANE	-275.48	-245.36	30.12
55	2,2-DIMETHYLHEPTANE	-288.2	-245.36	42.84
56	3-METHYLUNDECANE	-355.2	-325.98	29.22
57	ETHYLCYCLOPENTANE	-163.43	-137.96	25.47
58	cis-1,2-DIMETHYLCYCLOPENTANE	-165.27	-137.96	27.31
59	trans-1,3-DIMETHYLCYCLOPENTANE	-168.07	-137.96	30.11
60	n-PROPYLCYCLOPENTANE	-189.07	-164.84	24.23
61	1-METHYL-1-ETHYLCYCLOPENTANE	-193.8	-164.84	28.96
62	n-PROPYLCYCLOHEXANE	-237.4	-191.71	45.69
63	ISOPROPYLCYCLOHEXANE	-239.45	-191.71	47.74
64	1,1-DIETHYLCYCLOHEXANE	-277.11	-218.59	58.52
65	n-DECYLCYCLOHEXANE	-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-DIETHYLCYCLOHEXANE	-266.1	-218.59	47.51
69	2,6-DIMETHYLHEPTANE	-286.12	-245.36	40.76
70	2,2-DIMETHYL-3-ETHYLPENTANE	-272.7	-245.36	27.34
71	2,4-DIMETHYL-3-ETHYLPENTANE	-269.7	-245.36	24.34
72	1-TRIACONTENE	-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-HEPTENE	-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-NONENE	-148.8	-191.71	-42.91
102	1-UNDECENE	-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	-129.4	-164.84	-35.44
113	trans-3-OCTENE	-134.38	-164.84	-30.46
114	cis-4-OCTENE	-128.49	-164.84	-36.35
115	trans-4-OCTENE	-134.61	-164.84	-30.23
116	cis-3-OCTENE	-129.14	-164.84	-35.7
117	1-EICOSENE	-459.21	-487.33	-28.12
118	1-METHYLCYCLOPENTENE	-36.44	-57.44	-21
119	2,3-DIMETHYL-1-HEXENE	-136	-164.84	-28.84
120	1,4-DI-tert-BUTYLBENZENE	-188.9	-165.15	23.75
121	alpha-TOCOPHEROL	-873.4	-879.94	-6.54
122	1,2,3-TRIETHYLBENZENE	-130.32	-111.4	18.92
123	n-HEPTYLBENZENE	-140.6	-138.27	2.33
124	1,2,3,5-TETRAETHYLBENZENE	-196.36	-165.15	31.21
125	n-DECYLBENZENE	-217.5	-218.9	-1.4
126	PENTAETHYLBENZENE	-258.1	-218.9	39.2
127	m-TERPHENYL	165.58	156.52	-9.06
128	n-PENTYLBENZENE	-89.5	-84.52	4.98
129	n-HEXYLBENZENE	-115	-111.4	3.6
130	n-OCTYLBENZENE	-166.1	-165.15	0.95
131	n-NONYLBENZENE	-190.4	-192.02	-1.62
132	n-UNDECYLBENZENE	-241.18	-245.77	-4.59
133	n-TRIDECYLBENZENE	-288.73	-299.52	-10.79
134	n-TETRADECYLBENZENE	-311.49	-326.4	-14.91
135	n-DODECYLBENZENE	-264.79	-272.65	-7.86
136	2,3-DIMETHYL-2,3-DIPHENYLBUTANE	-59.68	-58.06	1.62
137	1,1,2-TRIPHENYLETHANE	130.2	102.77	-27.43
138	TETRAPHENYLMETHANE	247.1	182.98	-64.12
139	1,1,2,2-TETRAPHENYLETHANE	216	156.1	-59.9
140	1-(4-ETHYLPHENYL)-2-PHENYLETHANE	12.03	-4.32	-16.35
141	STYRENE	103.47	49.75	-53.72
142	1-n-NONYLNAPHTHALENE	-132.57	-111.76	20.81
143	1-n-DECYLNAPHTHALENE	-156.26	-138.64	17.62
144	1-n-HEXYL-1,2,3,4-TETRAHYDRONAPHTHALENE	-179.33	-165.25	14.08
145	1-PHENYLINDENE	148.61	129.85	-18.76
146	TRIPHENYLETHYLENE	233.38	156.41	-76.97
147	TETRAPHENYLETHYLENE	311.5	209.75	-101.75
148	trans-STILBENE	136.9	103.08	-33.82
149	ACENAPHTHALENE	186.6	183.65	-2.95
150	sec-BUTYLCYCLOHEXANE	-263.7	-218.59	45.11
151	PIMARIC ACID	-634.1	-611.29	22.81
152	ISOPIMARIC ACID	-670.4	-611.29	59.11
153	SULFUR DIOXIDE	-296.84	-315.26	-18.42
154	SULFUR TRIOXIDE	-441.04	-457.7	-16.66
155	ACETALDEHYDE	-166.4	-199.68	-33.28
156	PROPANAL	-215.3	-226.56	-11.26
157	1,2,3,6-TETRAHYDROBENZALDEHYDE	-162.1	-226.76	-64.66
158	BUTANAL	-239.2	-253.43	-14.23
159	HEPTANAL	-311.5	-334.06	-22.56
160	HEXANAL	-291.83	-307.18	-15.35
161	OCTANAL	-342.7	-360.93	-18.23
162	NONANAL	-367.93	-387.8	-19.87
163	2-ETHYLHEXANAL	-348.5	-360.93	-12.43
164	2-METHYLHEXANAL	-317.47	-334.06	-16.59
165	2-METHYL-2-PENTENAL	-201.8	-253.54	-51.74
166	2-ETHYL-2-HEXENAL	-244.6	-307.28	-62.68
167	DECANAL	-393.84	-414.68	-20.84
168	UNDECANAL	-419.06	-441.55	-22.49
169	DODECANAL	-445.25	-468.43	-23.18

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	-348.6	-334.06	14.54
182	4-HEPTANONE	-346.2	-334.06	12.14
183	3-HEXANONE	-320.2	-307.18	13.02
184	2-HEXANONE	-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	DIISOBUTYL KETONE	-408.5	-387.8	20.7
188	DIISOPROPYL 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-PROPIOLACTONE	-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-PROPANOL	-302.6	-280.2	22.4
205	ISOPROPANOL	-318.1	-280.2	37.9
206	1-BUTANOL	-327.2	-307.08	20.12
207	2-BUTANOL	-342.6	-307.08	35.52
208	2-METHYL-2-PROPANOL	-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-PROPANOL	-382.01	-333.95	48.06
213	1-HEXANOL	-377.5	-360.83	16.67
214	2-HEXANOL	-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-HEXANOL	-432.8	-414.58	18.22
218	2-METHYL-1-HEXANOL	-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-METHYLCYCLOHEXANOL	-388.17	-334.06	54.11
232	cis-2-METHYLCYCLOHEXANOL	-390.2	-334.06	56.14

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-BUTYL-CATECHOL	-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	TRIMETHYLOLPROPANE	-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-METHYLHEXANOIC 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

296	trans-CROTONIC ACID	-446.23	-395.88	50.35
297	STEARIC ACID	-948	-825.77	122.23
298	ACRYLIC ACID	-383.88	-369	14.88
299	OLEIC ACID	-802.49	-772.12	30.37
300	LINOLEIC ACID	-674.04	-718.48	-44.44
301	SALICYLIC ACID	-589.9	-511.66	78.24
302	ADIPIC ACID	-994.3	-841.82	152.48
303	MALEIC ACID	-789.4	-734.42	54.98
304	TEREPHTHALIC ACID	-816.18	-680.98	135.2
305	ACETIC ANHYDRIDE	-624.4	-591.97	32.43
306	PROPIONIC ANHYDRIDE	-679.1	-645.72	33.38
307	BUTYRIC ANHYDRIDE	-719.12	-699.47	19.65
308	PALUSTRIC ACID	-852.4	-664.94	187.46
309	SUCCINIC ANHYDRIDE	-607.8	-538.33	69.47
310	GLUTARIC ANHYDRIDE	-618.5	-565.2	53.3
311	PHTHALIC ANHYDRIDE	-460.1	-431.24	28.86
312	MALEIC ANHYDRIDE	-469.8	-484.68	-14.88
313	TRIMELLITIC ANHYDRIDE	-894.81	-796.66	98.15
314	METHYL FORMATE	-386.1	-395.78	-9.68
315	n-PROPYL FORMATE	-445.2	-449.52	-4.32
316	n-BUTYL FORMATE	-469.2	-476.4	-7.2
317	ISOBUTYL FORMATE	-475.87	-476.4	-0.53
318	n-PENTYL FORMATE	-493.28	-503.27	-9.99
319	n-OCTYL FORMATE	-566.45	-583.9	-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	-75.64
323	ETHYL ACETATE	-478.8	-449.52	29.28
324	n-PROPYL ACETATE	-504.32	-476.4	27.92
325	n-BUTYL ACETATE	-529.2	-503.27	25.93
326	ISOBUTYL ACETATE	-536.06	-503.27	32.79
327	ISOPENTYL ACETATE	-558.69	-530.15	28.54
328	ALLYL ACETATE	-386.3	-422.75	-36.45
329	ISOPROPYL ACETATE	-518.8	-476.4	42.4
330	sec-BUTYL ACETATE	-544.04	-503.27	40.77
331	VINYL ACETATE	-349.7	-395.88	-46.18
332	METHYL PROPIONATE	-463.3	-449.52	13.78
333	ETHYL PROPIONATE	-502.7	-476.4	26.3
334	n-PROPYL PROPIONATE	-527.5	-503.27	24.23
335	n-BUTYL PROPIONATE	-549.9	-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 ISOBUTYRATE	-564.5	-530.15	34.35
339	METHYL ACRYLATE	-362.2	-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 NONANOATE	-697.78	-691.4	6.38
343	n-BUTYL VALERATE	-613.3	-583.9	29.4
344	ETHYL ISOVALERATE	-570.9	-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	-446.7	-476.5	-29.8
348	DIOCTYL PHTHALATE	-1084.1	-1110.98	-26.88
349	DIISOCTYL PHTHALATE	-1087.3	-1110.98	-23.68
350	1,2-BENZENEDICARBOXYLIC ACID, HEPTYL, NONYL ESTER	-1085	-1110.98	-25.98
351	n-PENTYL ACETATE	-553	-530.15	22.85
352	2-ETHYLHEXYL ACETATE	-627.99	-610.77	17.22
353	BENZYL ACETATE	-368.8	-369.32	-0.52
354	ISOBUTYL ISOBUTYRATE	-594.07	-557.02	37.05
355	ISOPENTYL ISOVALERATE	-644.74	-610.77	33.97
356	METHYL OLEATE	-734.5	-799	-64.5
357	n-HEXYL ACETATE	-577.9	-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	DIISODECYL 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	DIISOBUTYL PHTHALATE	-890	-895.98	-5.98
367	DIMETHYL ISOPHTHALATE	-730.9	-734.73	-3.83
368	DI-n-DECYL PHTHALATE	-1197	-1218.48	-21.48
369	DI-n-UNDECYL PHTHALATE	-1248	-1325.98	-77.98
370	DI-n-HEXYL PHTHALATE	-987.8	-1003.48	-15.68
371	DIMETHYL TEREPHTHALATE	-732.6	-734.73	-2.13
372	DI-n-OCTYL TEREPHTHALATE	-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	n-BUTYL METHACRYLATE	-471.39	-503.38	-31.99
377	METHYL BENZOATE	-343.5	-342.44	1.06
378	ETHYL BENZOATE	-379.91	-369.32	10.59
379	DIETHYL CARBONATE	-682.65	-672.49	10.16
380	DIETHYL OXALATE	-806.28	-841.82	-35.54
381	DIETHYL MALONATE	-838.02	-868.69	-30.67
382	ISOPROPYL MYRISTATE	-820.33	-798.9	21.43
383	TRI-n-HEPTYL TRIMELLITATE	-1697	-1610.77	86.23
384	UNDECYL ESTER	-1137	-1164.73	-27.73
385	DIMETHYL ETHER	-184.1	-253.33	-69.23
386	DIETHYL ETHER	-279.4	-307.08	-27.68
387	DIISOPROPYL ETHER	-351.5	-360.83	-9.33
388	DI-n-BUTYL ETHER	-377.9	-414.58	-36.68
389	METHYL tert-BUTYL ETHER	-313.6	-333.95	-20.35
390	DI-sec-BUTYL ETHER	-401.5	-414.58	-13.08
391	METHYL ETHYL ETHER	-216.4	-280.2	-63.8
392	METHYL n-PROPYL ETHER	-265.89	-307.08	-41.19
393	ISOPROPYL BUTYL ETHER	-365.64	-387.7	-22.06
394	METHYL ISOBUTYL ETHER	-296.13	-333.95	-37.82
395	DI-n-HEXYL ETHER	-481.96	-522.07	-40.11
396	METHYL n-BUTYL ETHER	-290.6	-333.95	-43.35
397	ETHYL PROPYL ETHER	-303.59	-333.95	-30.36
398	1,4-DIOXANE	-355.1	-449.52	-94.42
399	TRIOXANE	-522.5	-618.74	-96.24
400	DI-tert-BUTYL ETHER	-399.61	-414.58	-14.97
401	DI-n-OCTYL ETHER	-582.75	-629.57	-46.82
402	DI-n-PENTYL ETHER	-425.12	-468.32	-43.2
403	METHYL sec-BUTYL ETHER	-305.24	-333.95	-28.71
404	tert-BUTYL ETHYL ETHER	-346.83	-360.83	-14
405	METHYL n-PENTYL ETHER	-315.1	-360.83	-45.73
406	ETHYL tert-PENTYL ETHER	-369.07	-387.7	-18.63
407	METHYLAL	-378.2	-476.3	-98.1
408	ACETAL	-491.41	-556.92	-65.51
409	ETHYL ISOBUTYL ETHER	-333.5	-360.83	-27.33
410	DI-n-PROPYL ETHER	-328.82	-360.83	-32.01
411	n-BUTYL ETHYL ETHER	-328.7	-360.83	-32.13
412	DIETHYLENE GLYCOL DI-n-BUTYL ETHER	-723.58	-914.26	-190.68
413	BENZYL ETHYL ETHER	-165.78	-226.87	-61.09
414	PHENETOLE	-152.6	-199.99	-47.39
415	1-METHYL-3-(METHYLETHOXY)BENZENE	-221.6	-253.74	-32.14
416	1,1-DIMETHOXYETHANE	-420.1	-503.17	-83.07
417	2,5-DIHYDROFURAN	-141.36	-199.79	-58.43
418	TETRAHYDROFURAN	-216.19	-253.43	-37.24
419	1-tert-BUTOXY-2-[2-(tert-BUTOXY)PROPOXY]PROPANE	-810.3	-968.01	-157.71

420	1,2-DIMETHOXYPROPANE	-422.3	-530.05	-107.75
421	sec-BUTYL-tert-BUTYL ETHER	-417.5	-414.58	2.92
422	ISOBUTYL-tert-BUTYL ETHER	-407	-414.58	-7.58
423	1,4-DICHLORO-trans-2-BUTENE	-112.53	-111.09	1.44
424	HEXACHLOROETHANE	-202.8	-218.48	-15.68
425	1,1,1,2-TETRACHLOROETHANE	-191	-164.73	26.27
426	1,1,2,2-TETRACHLOROETHANE	-194.6	-164.73	29.87
427	HEXACHLOROCYCLOPENTADIENE	-159.78	-138.17	21.61
428	PENTACHLOROETHANE	-187.6	-191.61	-4.01
429	3,4-DICHLORO-1-BUTENE	-106.91	-111.09	-4.18
430	DICHLORODIFLUOROMETHANE	-491.62	-487.37	4.25
431	TRICHLOROFLUOROMETHANE	-288.7	-312.61	-23.91
432	CHLOROTRIFLUOROMETHANE	-707.93	-662.12	45.81
433	2-CHLORO-1,1,1-TRIFLUOROETHANE	-741.8	-689	52.8
434	1,2-DICHLOROTETRAFLUROETHANE	-916.3	-917.5	-1.2
435	1,2-DIBROMOTETRAFLUROETHANE	-807.1	-917.5	-110.4
436	METHYL FLUORIDE	-234.3	-231.99	2.31
437	DIFLUOROMETHANE	-452.3	-433.62	18.68
438	TRIFLUOROMETHANE	-697.05	-635.25	61.8
439	CARBON TETRAFLUORIDE	-933.15	-836.88	96.27
440	ETHYL FLUORIDE	-264.4	-258.86	5.54
441	1,1,1-TRIFLUOROETHANE	-736.4	-662.12	74.28
442	DECAFLUROBUTANE	-2149.7	-2127.28	22.42
443	PERFLURO-n-DECANE	-4710	-4708.08	1.92
444	1,1-DIFLUOROETHYLENE	-328.96	-406.85	-77.89
445	TETRAFLUROETHYLENE	-658.56	-810.11	-151.55
446	BROMODIFLUOROMETHANE	-424.9	-460.49	-35.59
447	1,1-DIFLUOROETHANE	-497	-460.49	36.51
448	1-BROMOPROPANE	-121.8	-110.98	10.82
449	1-BROMOBUTANE	-143.8	-137.86	5.94
450	1-BROMOHEPTANE	-218.4	-218.48	-0.08
451	1,2-DIBROMOETHANE	-79.2	-110.98	-31.78
452	1,1,1-TRICHLOROTRIFLUOROETHANE	-822	-742.75	79.25
453	ISOPROPYL IODIDE	-74.8	-110.98	-36.18
454	2,2-DICHLORO-1,1,1-TRIFLUOROETHANE	-770.3	-715.87	54.43
455	HEXAFLUROPROPYLENE	-1079	-1240.24	-161.24
456	2-METHYL-2-AMINOBTUTANE	-171.4	-164.73	6.67
457	DI-n-PROPYLAMINE	-156.11	-191.61	-35.5
458	DIETHYLAMINE	-103.7	-137.86	-34.16
459	n-PROPYLAMINE	-101.47	-110.98	-9.51
460	n-PENTYLAMINE	-152.62	-164.73	-12.11
461	ISOBUTYLAMINE	-132.6	-137.86	-5.26
462	DIISOBUTYLAMINE	-218.5	-245.36	-26.86
463	PYRROLE	63.11	49.9	-13.21
464	METHYL DIETHANOLAMINE	-473.77	-556.92	-83.15
465	DIETHANOLAMINE	-493.8	-530.05	-36.25
466	TRIETHANOLAMINE	-667.35	-779.89	-112.54
467	sec-BUTYLAMINE	-137.49	-137.86	-0.37
468	tert-BUTYLAMINE	-150.6	-137.86	12.74
469	CYCLOHEXYLAMINE	-147.7	-137.96	9.74
470	HEXAMETHYLENEDIAMINE	-192.42	-218.48	-26.06
471	DIISOPROPYLAMINE	-178.5	-191.61	-13.11
472	DI-n-BUTYLAMINE	-206	-245.36	-39.36
473	PIPERIDINE	-86.4	-111.09	-24.69
474	QUINOLINE	141.22	130.11	-11.11
475	FORMANILIDE	-151.46	-146.35	5.11
476	1,2-PROPANEDIAMINE	-97.8	-137.86	-40.06
477	N-METHYLPYRROLE	62.38	23.03	-39.35
478	DIPHENYLAMINE	130	76.31	-53.69
479	HYDRACRYLONITRILE	-161.2	-199.79	-38.59
480	HYDROGEN CYANIDE	108.19	50.06	-58.13
481	ACETONITRILE	40.56	23.18	-17.38
482	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	-137.86	2.64
489	ISOBUTYL MERCAPTAN	-132	-137.86	-5.86
490	sec-BUTYL MERCAPTAN	-131	-137.86	-6.86
491	n-HEXYL MERCAPTAN	-175.7	-191.61	-15.91
492	n-NONYL MERCAPTAN	-248.66	-272.23	-23.57
493	n-OCTYL MERCAPTAN	-224.47	-245.36	-20.89
494	CYCLOHEXYL MERCAPTAN	-140.7	-137.96	2.74
495	METHYL ETHYL SULFIDE	-91.6	-110.98	-19.38
496	METHYL n-PROPYL SULFIDE	-118.5	-137.86	-19.36
497	METHYL t-BUTYL SULFIDE	-157.1	-164.73	-7.63
498	DI-n-PROPYL SULFIDE	-169.9	-191.61	-21.71
499	ETHYL n-OCTYL SULFIDE	-273.3	-299.11	-25.81
500	DIMETHYL SULFIDE	-65.4	-84.11	-18.71
501	THIOPHENE	80.2	49.9	-30.3
502	DIETHYL DISULFIDE	-120.1	-164.73	-44.63
503	UNDECYL MERCAPTAN	-302.87	-325.98	-23.11
504	n-DECYL MERCAPTAN	-276.5	-299.11	-22.61
505	n-PENTYL MERCAPTAN	-149.69	-164.73	-15.04
506	DICYCLOHEXYL SULFIDE	-241.8	-245.56	-3.76
507	THIAINDAN	59.26	22.87	-36.39
508	n-DODECYL MERCAPTAN	-327.18	-352.86	-25.68
509	tert-OCTYL MERCAPTAN	-245.23	-245.36	-0.13
510	n-HEPTYL MERCAPTAN	-200.5	-218.48	-17.98
511	n-BUTYL MERCAPTAN	-124.7	-137.86	-13.16
512	TETRAHYDROTHIOPHENE	-72.9	-84.21	-11.31
513	DIMETHYL SULFOXIDE	-204.2	-226.56	-22.36
514	3-METHYL SULFOLANE	-488	-395.98	92.02
515	DI-n-BUTYL SULFONE	-609.86	-530.25	79.61
516	ACETYL CHLORIDE	-272.8	-226.56	46.24
517	CHLOROACETIC ACID	-510.5	-422.65	87.85
518	CHLOROACETYL CHLORIDE	-283.7	-253.43	30.27
519	TRICHLOROACETYL CHLORIDE	-280.8	-307.18	-26.38
520	BENZOYL CHLORIDE	-158	-146.35	11.65
521	p-CHLOROBENZOTRIFLUORIDE	-663.63	-608.79	54.84
522	2,4-DICHLOROBENZOTRIFLUORIDE	-702.75	-635.66	67.09
523	FLUOROBENZENE	-150.6	-151.78	-1.18
524	3-CHLORO-1,2-PROPANEDIOL	-525.3	-503.17	22.13
525	1,3-DICHLORO-2-PROPANOL	-385.3	-333.95	51.35
526	2,3-DICHLORO-1-PROPANOL	-381.5	-333.95	47.55
527	DI(2-CHLOROETHYL)ETHER	-356.2	-360.83	-4.63
528	3-(METHYLMERCAPTO)PROPANAL	-211.1	-280.31	-69.21
529	TRIFLUOROACETIC ACID	-1069.9	-1000.66	69.24
530	GLYCINE	-528.1	-422.65	105.45
531	4-METHOXYPHENYLACETIC ACID	-578.4	-565.41	12.99
532	N,N-DIMETHYLFORMAMIDE	-239.2	-253.43	-14.23
533	2-METHACRYLAMIDE	-269.68	-226.66	43.02
534	ACRYLAMIDE	-212.08	-199.79	12.29
535	epsilon-CAPROLACTAM	-328.5	-280.41	48.09
536	HEXAMETHYL PHOSPHORAMIDE	-533.9	-414.68	119.22
537	ACETALDOL	-433.62	-449.52	-15.9
538	FURFURAL	-201.6	-288.64	-87.04
539	CARBONYL SULFIDE	-142	-146.04	-4.04
540	PHOSGENE	-218.9	-226.56	-7.66
541	ACETOMETHOXANE	-873.7	-895.57	-21.87
542	ETHYLENE GLYCOL DIACRYLATE	-662.81	-788.27	-125.46
543	PROPYLENE GLYCOL MONOMETHYL ETHER ACETATE	-663.23	-699.37	-36.14
544	DIPROPYLENE GLYCOL MONOMETHYL ETHER ACETATE	-878.99	-976.09	-97.1

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	HEXAMETHYLCYCLOTTRISILOXANE	-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]TRIETHOXSILANE	-1054	-1153.96	-99.96
553	3-(TRIMETHOXSILYL)-1-PROPANETHIOL	-933.1	-1073.34	-140.24
554	OCTAMETHYLCYCLOTETRASILOXANE	-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-METHYLBENZYL 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-OCTYLPHENOL	-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

608	IBUPROFEN	-559.53	-476.82	82.71
609	METHYL MALEIC ANHYDRIDE	-504.55	-511.56	-7.01
610	sec-BUTYL FORMATE	-482.76	-476.4	6.36
611	tert-BUTYL FORMATE	-499.65	-476.4	23.25
612	n-HEXYL FORMATE	-518.49	-530.15	-11.66
613	n-HEPTYL FORMATE	-542.98	-557.02	-14.04
614	CYCLOHEXYL FORMATE	-495.52	-476.5	19.02
615	tert-BUTYL ACETATE	-561.02	-503.27	57.75
616	METHYL ISOBUTYRATE	-501.76	-476.4	25.36
617	ETHYL ISOBUTYRATE	-538.74	-503.27	35.47
618	ISOPROPYL ACRYLATE	-419.4	-449.63	-30.23
619	BENZYL FORMATE	-305.13	-342.44	-37.31
620	CETYL METHACRYLATE	-742.81	-825.87	-83.06
621	DIMETHYL-2,6-NAPHTHALENEDICARBOXYLATE	-709.5	-654.47	55.03
622	CYCLOHEXYL ACETATE	-553.48	-503.38	50.1
623	n-NONYL n-UNDECYL PHTHALATE	-1140	-1218.48	-78.48
624	DIISONONYL PHTHALATE	-1237	-1164.73	72.27
625	DIETHYL PHTHALATE	-776.6	-788.48	-11.88
626	DIMETHYL PHTHALATE	-677.81	-734.73	-56.92
627	DIETHYL SUCCINATE	-913.07	-895.57	17.5
628	DIHEXYL ADIPATE	-1161.6	-1164.31	-2.71
629	ETHYLIDENE DIACETATE	-865.97	-841.82	24.15
630	DIBUTYL MALEATE	-772.2	-949.42	-177.22
631	METHYL DODECANOATE	-693	-691.4	1.6
632	DIETHYL MALEATE	-798.18	-841.92	-43.74
633	DIMETHYL MALEATE	-680.85	-788.17	-107.32
634	DIPROPYL MALEATE	-785.11	-895.67	-110.56
635	sec-BUTYL ACRYLATE	-436.8	-476.5	-39.7
636	VINYL PIVALATE	-429.1	-476.5	-47.4
637	DIMETHYL CARBONATE	-607.27	-618.74	-11.47
638	n-PROPYL BENZOATE	-397.7	-396.19	1.51
639	ETHYL ISOPROPYL ETHER	-315.8	-333.95	-18.15
640	ETHYL n-HEXYL ETHER	-381.01	-414.58	-33.57
641	1,3-DIOXANE	-377.5	-449.52	-72.02
642	1,2-DIETHOXYETHANE	-451.43	-556.92	-105.49
643	2,3-DICHLOROPROPENE	-73.3	-84.21	-10.91
644	n-PENTADECYLBENZENE	-335.24	-353.27	-18.03
645	n-HEXADECYLBENZENE	-414.67	-380.15	34.52
646	n-HEPTADECYLBENZENE	-442.5	-407.02	35.48
647	n-OCTADECYLBENZENE	-469.9	-433.89	36.01
648	1,3-DICHLOROHEXAFLUOROPROPANE	-1321.8	-1347.63	-25.83
649	1,2-DICHLOROHEXAFLUOROCYCLOBUTANE	-1282.7	-1320.86	-38.16
650	3,3,3-TRIFLUOROPROPENE	-614.2	-635.35	-21.15
651	1,1,2-TRIFLUOROETHANE	-675.9	-662.12	13.78
652	PERFLUORO-n-HEXADECANE	-7251	-7288.88	-37.88
653	PERFLUOROMETHYLCYCLOPENTANE	-2533	-2530.64	2.36
654	1,1,1,2,2-PENTAFLUOROPROPANE	-1111	-1092.26	18.74
655	1,1,1,2,3,3-HEXAFLUOROPROPANE	-1333	-1293.89	39.11
656	BENZOTRIFLUORIDE	-636.7	-581.91	54.79
657	2-BROMOBUTANE	-155.1	-137.86	17.24
658	BROMOCHLOROMETHANE	-76.01	-84.11	-8.1
659	HALOTHANE	-720	-715.87	4.13
660	1,2-DIFLUOROETHANE	-447.7	-460.49	-12.79
661	PENTACHLOROFLUROETHANE	-382	-393.24	-11.24
662	1,2-DICHLORO-1,1,2-TRIFLUOROETHANE	-735.55	-715.87	19.68
663	2-CHLORO-1,1,1,2-TETRAFLUROETHANE	-924.7	-890.63	34.07
664	1,1-DICHLORO-1-FLUROETHANE	-366.4	-312.61	53.79
665	1,1,1,2-TETRAFLUROETHANE	-895.79	-863.75	32.04
666	HEXAFLUROACETONE	-1460	-1436.33	23.67
667	OCTAFLUROOPROPANE	-1783.2	-1697.14	86.06
668	OCTAFLUROO-2-BUTENE	-1648	-1670.37	-22.37
669	OCTAFLUROOCYCLOBUTANE	-1528	-1670.37	-142.37
670	1,1,1-TRICHLOROFLUROETHANE	-337.1	-339.49	-2.39

671	1,1,2,2-TETRAFLUOROETHANE	-892.4	-863.75	28.65
672	p-BROMOTOLUENE	17.14	-3.9	-21.04
673	n-HEXYL IODIDE	-146.4	-191.61	-45.21
674	BROMOTRIFLUOROMETHANE	-648.98	-662.12	-13.14
675	DIBROMODIFLUOROMETHANE	-386.6	-487.37	-100.77
676	CHLOROTRIFLUOROETHYLENE	-555.3	-635.35	-80.05
677	HEXAFLUROETHANE	-1343.9	-1267.01	76.89
678	1-CHLORO-1,1-DIFLUOROETHANE	-529.7	-487.37	42.33
679	n-HEXYLAMINE	-177.12	-191.61	-14.49
680	n-HEPTYLAMINE	-201.33	-218.48	-17.15
681	n-OCTYLAMINE	-226.02	-245.36	-19.34
682	n-NONYLAMINE	-250.44	-272.23	-21.79
683	n-DECYLAMINE	-275.19	-299.11	-23.92
684	n-DODECYLAMINE	-368.18	-352.86	15.32
685	CYCLOHEXYL ISOCYANATE	-200.64	-253.64	-53
686	N,N'-DI-tert-BUTYLETHYLENEDIAMINE	-264.9	-325.98	-61.08
687	DICYCLOHEXYLAMINE	-246.4	-245.56	0.84
688	N-METHYLCYCLOHEXYLAMINE	-149.52	-164.84	-15.32
689	N-AMINOETHYL ETHANOLAMINE	-280.19	-360.83	-80.64
690	PHENYL ISOCYANATE	-61.08	-92.7	-31.62
691	ISOQUINOLINE	134.2	130.11	-4.09
692	p-AMINODIPHENYL	81	76.31	-4.69
693	2,6-DIETHYLANILINE	-84.23	-84.52	-0.29
694	3-METHYLPYRIDINE	61.9	22.97	-38.93
695	4-METHYLPYRIDINE	59.2	22.97	-36.23
696	ETHYL t-BUTYL SULFIDE	-187.3	-191.61	-4.31
697	tert-NONYL MERCAPTAN	-266.22	-272.23	-6.01
698	2-METHYLTHIOPHENE	44.6	23.03	-21.57
699	3-METHYLTHIOPHENE	43.1	23.03	-20.07
700	CAMPHOR	-319.4	-307.39	12.01
701	N-METHYLFORMAMIDE	-241.48	-226.56	14.92
702	DIACETONE ALCOHOL	-592.79	-503.27	89.52
703	FURFURYL ALCOHOL	-276.2	-342.29	-66.09
704	N,N-DIMETHYLACETAMIDE	-278.3	-280.31	-2.01
705	ACETAMINOPHEN	-396.04	-369.32	26.72
706	p-METHOXYPHENOL	-335.51	-369.21	-33.7
707	2-METHOXYETHANOL	-416.32	-476.3	-59.98
708	2-ETHOXYETHANOL	-448.22	-503.17	-54.95
709	2-BUTOXYETHANOL	-497.4	-556.92	-59.52
710	2-(2-METHOXYETHOXY)ETHANOL	-589.99	-726.14	-136.15
711	2-(2-ETHOXYETHOXY)ETHANOL	-626.28	-753.01	-126.73
712	2-AMINOETHOXYETHANOL	-438.01	-530.05	-92.04
713	ETHYLCHLOROACETATE	-509.3	-476.4	32.9
714	2-(2-(2-METHOXYETHOXY)ETHOXY)ETHANOL	-786.4	-975.98	-189.58
715	SUCCINIMIDE	-460.25	-369.11	91.14
716	4-CARBOXYBENZALDEHYDE	-544.91	-484.89	60.02
717	THIOGLYCOLIC ACID	-454.56	-422.65	31.91
718	2-HYDROXYETHYL METHACRYLATE	-576.15	-645.72	-69.57
719	METHYL LACTATE	-643.1	-645.62	-2.52
720	2-METHOXY PROPANOL-1	-449.47	-503.17	-53.7
721	alpha-METHYLBENZYL ALCOHOL FORMATE	-347.1	-369.32	-22.22
722	2-FORMYL BENZOIC ACID	-531.54	-484.89	46.65
723	2-HYDROXYACETOPHENONE	-342.2	-342.44	-0.24
724	4-HYDROXYACETOPHENONE	-364.3	-342.44	21.86
725	4-HYDROXYSTYRENE	-109.67	-146.35	-36.68
726	ACETYLSALICYLIC ACID	-815.6	-707.86	107.74
727	p-PHENETIDINE	-172.6	-226.87	-54.27
728	ACETOL	-414.15	-422.65	-8.5
729	o-CHLOROPHENOL	-172.35	-173.12	-0.77
730	1-ISOPROPOXY-2-PROPANOL	-529.6	-556.92	-27.32
731	ISOPHTHALOYL CHLORIDE	-367.5	-342.55	24.95
732	4-FORMYLMORPHOLINE	-369.9	-449.63	-79.73
733	FLUOSULFONIC ACID	-795.78	-712.98	82.8

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	-8.22
740	2-METHYL-1-TRIDECANOL	-566.9	-575.82	-8.92
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-NONENE	-188.7	-218.59	-29.89
750	8-METHYL-1-NONENE	-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-CROTYL ACETATE	-410.1	-449.63	-39.53
757	sec-BUTENYL ACETATE	-409	-449.63	-40.63
758	VINYLETHYLENE CARBONATE	-555.4	-565.2	-9.8
759	DIOCTYL 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	TRIFLUOROIODOMETHANE	-589.1	-662.12	-73.02
764	DIFLUOROMETHYL TRIFLUOROMETHYL ETHER	-1316	-1261.47	54.53
765	CYCLOPROPANECARBOXAMIDE	-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	NIACIN	-344.9	-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-METHYLTHIACYCLOPENTANE	-105	-111.09	-6.09
780	METHYL ISOPROPYL SULFIDE	-123.5	-137.86	-14.36
781	2-ETHYLTHIOPHENE	16.61	-3.85	-20.46
782	2-n-PROPYLTHIOPHENE	-8.96	-30.72	-21.76
783	ETHYL PROPYL DISULFIDE	-146.2	-191.61	-45.41
784	DIISOPENTYLSULFIDE	-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	DIPROPYLENE 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-(2-BUTOXYETHOXY)ETHOXY)ETHANOL	-844.47	-1056.61	-212.14
795	2-(2-(2-ETHOXYETHOXY)ETHOXY)ETHANOL	-796.01	-1002.86	-206.85
796	2-HEXOXYETHANOL	-560.3	-610.67	-50.37

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 MONOETHYL ETHER	-721.6	-806.76	-85.16
809	TRIPROPYLENE GLYCOL MONOETHYL 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	-435.55	-377.56	57.99
817	FEROUS CHLORIDE	-341.83	-350.69	-8.86
818	FERRIC CHLORIDE	-399.41	-377.56	21.85
819	DIMETHYLCHLOROSILANE	-326.35	-377.56	-51.21
820	TRIMETHYLCHLOROSILANE	-382.61	-404.43	-21.82
821	DIMETHYLDICHLOROSILANE	-480.4	-404.43	75.97
822	DIPHENYLDICHLOROSILANE	-238	-244.02	-6.02
823	DICHLORODIETHYLSILANE	-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	-449.52	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	VINYLTRIMETHOXYSILANE	-835.9	-965.94	-130.04
842	TRIMETHOXYSILANE	-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	TARTARIC ACID	-1289.5	-1180.25	109.25

860	HYDROXYCAPROIC ACID	-794.19	-699.37	94.82
861	ETHYL LACTATE	-695.08	-672.49	22.59
862	2-ETHOXYETHYL ACETATE	-663	-699.37	-36.37
863	DIETHYLENE GLYCOL ETHYL ETHER ACETATE	-833.64	-949.21	-115.57
864	METHYL ACETOACETATE	-642.4	-618.85	23.55
865	ETHYL ACETOACETATE	-612.24	-645.72	-33.48
866	METHYL CYANOACETATE	-298.3	-369.11	-70.81
867	ETHYL CYANOACETATE	-386.49	-395.98	-9.49
868	ETHYL HYDROGEN SULFATE	-887.3	-761.19	126.11
869	ACRYLOXY PROPIONIC ACID	-786.6	-788.17	-1.57
870	THIODIGLYCOL	-477.92	-530.05	-52.13
871	2-MERCAPTOETHANOL	-248.94	-280.2	-31.26
872	ETHYLTHIOETHANOL	-290.46	-333.95	-43.49
873	DIETHYLETHANOLAMINE	-309.5	-387.7	-78.2
874	DIMETHYLETHANOLAMINE	-256.97	-333.95	-76.98
875	DIISOPROPANOLAMINE	-572.82	-583.79	-10.97
876	3-METHOXYISOPROPYLAMINE	-256.2	-333.95	-77.75
877	ETHYLENE GLYCOL MONOBUTYL ETHER ACETATE	-710.3	-753.12	-42.82
878	ETHYL VANILLIN	-532.3	-565.41	-33.11
879	2-HYDROXYETHYL ACRYLATE	-559.87	-618.85	-58.98
880	ETHYL-3-ETHOXYPROPIONATE	-684.7	-726.24	-41.54
881	BIS-(2-HYDROXYETHYL) TEREPHTHALATE	-1200	-1180.67	19.33
882	DI-(2-CHLOROETHOXY)METHANE	-536.2	-583.79	-47.59
883	1-METHYL VINYL ACETATE	-390.1	-422.75	-32.65
884	2-PENTOXYETHANOL	-528.2	-610.67	-82.47
885	1-CHLORO-3-PROPANOL	-343.7	-307.08	36.62
886	TRIFLUOROACETAMIDE	-935.3	-831.45	103.85
887	DILACTIDE (dl)	-792.1	-788.17	3.93
888	2-(2-PENTOXYETHOXY)ETHANOL	-725.7	-833.64	-107.94
889	METHYL-4-FORMYLBENZOATE	-476.1	-511.76	-35.66
890	HYDROXYPIVALYL HYDROXYPIVALATE	-1003	-1002.96	0.04
891	TETRAETHYLENE GLYCOL MONOBUTYL ETHER	-1032	-1306.45	-274.45
892	METHYL para-TOLUATE	-390.7	-369.32	21.38

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 ΔH_f° by the Eq. (2) for test set as an excluded data set.

ID	Name	ΔH_f° (kJ/mol)		Res
		DIPPR 801	Calculated from Eq. (2)	
1	2-METHYLPENTANE	-204.64	-164.73	39.91
2	2-METHYLHEXANE	-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-TETRAMETHYLBUTANE	-268.61	-218.48	50.13
8	2,2,5-TRIMETHYLHEXANE	-293.3	-245.36	47.94
9	2,2,3,4-TETRAMETHYLPENTANE	-277.7	-245.36	32.34
10	2,3,3,4-TETRAMETHYLPENTANE	-277.9	-245.36	32.54
11	2,2,3,3-TETRAMETHYLHEXANE	-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-EICOSANE	-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

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-PROPANOL	-334.7	-307.08	27.62
68	2-METHYL-2-BUTANOL	-379.5	-333.95	45.55
69	2-METHYL-1-PENTANOL	-383.8	-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-METHYLCYCLOHEXANOL	-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

89	p-CRESOL	-199.28	-173.12	26.16
90	TRIETHYLENE GLYCOL	-804.2	-949.11	-144.91
91	NEOPENTYL GLYCOL	-551.2	-530.05	21.15
92	TRIPROPYLENE GLYCOL	-921.41	-1029.73	-108.32
93	1,2,3-BUTANETRIOL	-764.1	-699.26	64.84
94	1,2,4-BUTANETRIOL	-745.1	-699.26	45.84
95	1,4-BUTANEDIOL	-503.3	-503.17	0.13
96	INOSITOL	-1362.1	-1287.65	74.45
97	2-METHYLBUTYRIC ACID	-554.5	-476.4	78.1
98	n-TRIDECANOIC ACID	-806.6	-691.4	115.2
99	n-TETRADECANOIC ACID	-833.5	-718.27	115.23
100	cis-CROTONIC ACID	-347.27	-395.88	-48.61
101	2-METHYLOCTANOIC ACID	-661.6	-583.9	77.7
102	METHACRYLIC ACID	-408.09	-395.88	12.21
103	BENZOIC ACID	-385.2	-315.57	69.63
104	o-TOLUIC ACID	-416.5	-342.44	74.06
105	PHTHALIC ACID	-782.07	-680.98	101.09
106	ISOPHTHALIC ACID	-803	-680.98	122.02
107	ETHYL FORMATE	-420.5	-422.65	-2.15
108	METHYL ACETATE	-445.8	-422.65	23.15
109	n-PROPYL n-BUTYRATE	-554.1	-530.15	23.95
110	METHYL n-BUTYRATE	-490	-476.4	13.6
111	n-BUTYL ACRYLATE	-433.45	-476.5	-43.05
112	BENZYL BENZOATE	-273.1	-289.11	-16.01
113	ETHYLENE CARBONATE	-586.3	-565.1	21.2
114	n-NONYL ACETATE	-654.12	-637.65	16.47
115	2-ETHYLHEXYL ACRYLATE	-526.06	-584	-57.94
116	ETHYLENE GLYCOL DIACETATE	-865.43	-841.82	23.61
117	ISOBUTYL METHACRYLATE	-465.16	-503.38	-38.22
118	METHYL DECANOATE	-640.5	-637.65	2.85
119	DIMETHYL-1,4-CYCLOHEXANEDICARBOXYLATE	-948.9	-895.67	53.23
120	METHYL ISOPROPYL ETHER	-278.7	-307.08	-28.38
121	METHYL tert-PENTYL ETHER	-339.86	-360.83	-20.97
122	ISOPROPYL ISOBUTYL ETHER	-370.63	-387.7	-17.07
123	DIETHYLENE GLYCOL DIETHYL ETHER	-638.4	-806.76	-168.36
124	2,3,4,5,2',3',4',5'-OCTAHYDRO-BIFURYL-(3,3')	-390.5	-503.38	-112.88
125	CARBON TETRACHLORIDE	-128.41	-137.86	-9.45
126	3-CHLOROPROPENE	-30.8	-57.34	-26.54
127	1,4-DICHLORO-cis-2-BUTENE	-105.65	-111.09	-5.44
128	m-CHLOROBENZOYL CHLORIDE	-189.7	-173.22	16.48
129	1,3-DICHLORO-trans-2-BUTENE	-122.25	-111.09	11.16
130	CHLOROFLUOROMETHANE	-264	-258.86	5.14
131	CHLORODIFLUOROMETHANE	-481.6	-460.49	21.11
132	2-CHLORO-1,1-DIFLUOROETHYLENE	-329	-433.72	-104.72
133	PERFLUORO-n-OCTANE	-3860	-3847.81	12.19
134	METHYL BROMIDE	-37.7	-57.23	-19.53
135	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	DICHLOROFLUOROMETHANE	-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 t-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	BIS[3-(TRIETHOXSILYL)PROPYL]DISULFIDE	-2158	-2304.44	-146.44
162	3-NONANONE	-397.4	-387.8	9.6
163	4-NONANONE	-398.3	-387.8	10.5
164	2,6,8-TRIMETHYL-4-NONANONE	-490.9	-468.43	22.47
165	2,7-DIMETHYLOCTANE	-311.3	-272.23	39.07
166	1-PHENYL-2-PROPANOL	-220.17	-226.87	-6.7
167	2-PHENYL-1-PROPANOL	-223	-226.87	-3.87
168	p-TOLUALCOHOL	-209.27	-199.99	9.28
169	DINONYLPHENOL	-682.28	-629.99	52.29
170	CITRACONIC ACID	-824.46	-761.3	63.16
171	2-ETHYL BUTYRIC ACID	-599.99	-503.27	96.72
172	PROPYLENE CARBONATE	-613.2	-591.97	21.23
173	GLYCERYL TRIACETATE	-1330.8	-1260.98	69.82
174	DI-n-BUTYL PHTHALATE	-842.6	-895.98	-53.38
175	ISOBUTYL ACRYLATE	-438.95	-476.5	-37.55
176	DIISOBUTYL ETHER	-387.92	-414.58	-26.66
177	ETHYLAL	-450.41	-530.05	-79.64
178	PERFLUORO-n-PENTANE	-2608	-2557.41	50.59
179	PERFLUORO-n-HEPTANE	-3338	-3417.68	-79.68
180	1,1,1,2,3,3,3-HEPTAFLUOROPROPANE	-1552	-1495.51	56.49
181	2,2-DICHLORO-1,1,2-TRIFLUOROETHANE	-728.38	-715.87	12.51
182	1,1,2-TRICHLOROTRIFLUOROETHANE	-805.8	-742.75	63.05

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 DIISOCYANATE	-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	FEROUS 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 DIISOBUTYRATE	-1118	-1110.56	7.44
202	DIMETHYL SUCCINATE	-845.1	-841.82	3.28
203	BENZENE-1,2,4-TRICARBOXYLIC ACID TRIMETHYL ESTER	-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	DIPROPYLENE GLYCOL n-PROPYL ETHER	-737.7	-833.64	-95.94
212	CROTYL GLYCOL ETHER	-386.6	-503.27	-116.67
213	DIETHYLSULFITE	-600.43	-672.49	-72.06
214	DIMETHYLDIMETHOXSILANE	-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	TRIDECAFLUROHEPTANOIC ACID	-3215	-3151.33	63.67
219	tert-BUTYLFORMAMIDE	-340.98	-307.18	33.8
220	METHYLETHANOLAMINE	-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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