## OPTIMAL DESCRIPTORS BASED ON EXTENDED CONNECTIVITY AND CODES OF CYLES: QSPR OF HYDROCARBON NORMAL BOILING POINTS

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**ABSTRACT:** (0, 1)-codes reflected presence / absence of six- and fivemembers cycles produce considerable improving statistical characteristics of quantitative structure–property relationships between optimal descriptors and normal boiling points of alkanes, alkylbenzenes, and polyaromatic hydrocarbons.

Keywords: QSPR, normal boiling points, hydrocarbons, cycle code, optimal descriptors

#### **INTRODUCTION**

Our real world is rather uncertain. Suppose we are carrying out a chemical reaction, which allows us to obtain a product. In the very beginning we observe a complete uncertainty regarding the molecule. In fact, we have no information about its composition, the constitution of the molecular skeleton, its stereochemical features, its physical properties and biological activities and so on. Gradually, performing routine suitable experiments, we gather data. Then the acquisition of the structural information is complete there is no uncertainty, at least about its structure. The information about a real physical system is a measure of decreasing uncertainty of the system by means of some physical activities.

We can define knowledge as the perception of the logical relations among the structures of the information. Any systematic treatment of information needs some previous knowledge. Therefore, research is always an iterative process, as depicted in Scheme 1 [1].

**SCHEME 1** 



The central problem in theory of Quantitative Structure Property-Activity Relationships (QSPR/QSAR) is to convert chemical structures in to mathematical molecular descriptors that are relevant to the physico-chemical property or to the mechanism of the biological activity. Topological indices are among the best descriptors, although there are other sort of them, such as Molecular Orbital indices and other properties/activities which are also employed in these studies. It is a well known fact that molecular structure is one of the basic concepts of chemistry since properties and molecular behavior follow from their structures. In particular, properties of a molecule are a consequence of a complicated interplay of its topology (i.e. atomic connectivity), metric characteristics (bond lengths, valence and torsional angles) and detailed dynamics of electrons and nuclei. Finding out how various molecular features depend on molecular structure is one of the central fields of chemistry and particularly the main subject of QSAR/QSPR studies [2].

The topological indices are those structure molecular descriptors derived from a graph theoretical representation of molecules. These molecular descriptors should carry out most of the desired attributes for topological indices. Flexible topological descriptors make up a quite efficient set of variables to employ in QSAR/QSPR studies which have been employed successfully in many cases to predict physico-chemical properties and biological activities [3-10].

In a recent study **[11]** on the comparison of QSPR models based on hydrogen-filled graphs and on graphs of atomic orbitals, optimal descriptors have been calculated without taking into account the presence/absence of cycles in the molecular structure. The aim of the present study is to estimate the efficacy of codes of six- and five-member cycles in constructing optimal descriptors in order to get a better molecular description. We have chosen a set of 140 hydrocarbons to predict their normal boiling points.

#### **METHOD**

Descriptors used in the present study have been calculated as

<sup>1</sup>DCW(a<sub>k</sub>,EC<sub>k</sub>) = { 
$$\sum_{k=1}^{n} CW(a_k) + \sum_{k=1}^{n} CW(^{x}EC_k)$$
 }<sup>m</sup> (1)

<sup>2</sup>DCW(a<sub>k</sub>,EC<sub>k</sub>) = { CW(CC) + 
$$\sum_{k=1}^{n}$$
 CW(a<sub>k</sub>) +  $\sum_{k=1}^{n}$  CW(<sup>x</sup>EC<sub>k</sub>) }<sup>m</sup> (2)

where:

 $a_k$  is chemical element (C or H) in hydrogen-filled molecular graph (HFG) that is presented by k-th vertex in the graph,

<sup>x</sup>EC<sub>k</sub> is the extended connectivity of x-th order (x = 0,1,2),

CC is the code of cycles, and they were calculated as shown in Table 1,

 $CW(a_k)$  is the correlation weight of presence  $a_k$  in HFG,

 $CW(^{x}EC_{k})$  is the correlation weight for a given extended connectivity value,

CW(CC) is the correlation weight of the code of cycles,

n is the number of vertex in the HFG, and

$$m = 0.5$$
.

Numerical data on the  $CW(a_k)$ ,  $CW({}^xEC_k)$ , and CW(CC) have been calculated via Monte Carlo optimization method, i.e., we look for those values of the CWs producing maximal correlation coefficient between <sup>q</sup>DCW and normal boiling points (NBPs) of hydrocarbon of the training set have been obtained by the corresponding optimization procedure. From the data one can then calculate the desired physical chemistry property by the Least Square method NBP model

$$NBP = C_0 + C_1 {}^{q}DCW(a_k, EC_k)$$
(3)

Predictive potential of the model must be validated with an external test set. Recently these hydrocarbons have been examined in Ref. 11. We have resorted to the splitting of the whole molecular set into a training and a test set from the study. Choice of m = 0.5 is based on fact that often correlation between normal boiling points and descriptors are non linear [12,13]. We have tested m = 1 and m = 0.5. Statistical characteristics in case of m = 0.5 were better than those corresponding to m = 1. Details on models with m = 1 will not be examined further in this paper. Calculation of the extended connectivity of increasing orders has been described in Ref. 14. Version of the Cycle codes (CC) are shown in Table 1 and it is a particular case of the generalized CC definition used in [15].

#### **RESULTS AND DISCUSSION**

From Table 2 one can see that <sup>2</sup>DCW modeling gives a model of normal boiling points of better statistical quality than <sup>1</sup>DCW modeling. Correlation weights, obtained in three probes of the Monte Carlo optimization, for calculation of the <sup>2</sup>DCW, are shown in Table 3. Calculation of the <sup>2</sup>DCW( $a_k$ , <sup>1</sup>EC\_k) for m-xylene is shown in Table 4. The model of the hydrocarbon normal boiling points obtained in first probe of the optimization is the following

NBP = 
$$-448.8 + 117.52 * {}^{2}DCW(a_{k}, {}^{1}EC_{k})$$
 (4)

 $n = 70, r^2 = 0.9988, s = 5.86, F = 57619$  (training set)  $n = 70, r^2 = 0.9990, s = 4.82, F = 68071$  (test set)

The results derived from this model is displayed graphically for training and test sets in Figures 1 and 2, respectively. This model is slightly better than one described in [11], but the it is considerably simpler than the previous one.

### CONCLUSIONS

We have shown that utilization of the described cycle codes produce considerable improving statistical quality models of hydrocarbon normal boiling points regarding those calculation which do not take into account the presence of such cycles. In order to get a better conclusion on the goodness of the method proposed here, it is necessary to perform complementary calculations on other physicochemical properties and biological activities for other sets of molecules. Work along these lines are currently under development and results will be presented elsewhere in the forthcoming future.

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Situation in molecular structure	Numerical value of the CC
There is no cycle	C00
Six member cycle (one or more)	C10
Five member cycle (one or more)	C01
Both six-member and five-member cycles	C11

**Table 1.** Definition of the (0,1) cycle codes (CC).

 Table 2. Statistical characteristics on the <sup>1</sup>DCW- and <sup>2</sup>DCW-modeling.

Probe		N <sub>op</sub> *	<b>C</b> <sub>1</sub>	C <sub>0</sub>	$\mathbf{r}^2$	s, <sup>0</sup> C	F	$\mathbf{r}^2$	s, <sup>0</sup> C	F
DCW-modeling										
1	<sup>0</sup> EC	5	50.759	-378.100	0.9917	15.526	8140	0.9935	12.595	10351
2			56.014	-378.098	0.9917	15.526	8140	0.9935	12.596	10351
3			53.229	-378.123	0.9917	15.526	8140	0.9935	12.595	10353
1	<sup>1</sup> EC	10	79.442	-364.654	0.9958	11.065	16092	0.9958	9.874	16260
2			86.660	-364.808	0.9958	11.065	16092	0.9958	9.874	16262
3			81.802	-364.789	0.9958	11.065	16092	0.9958	9.877	16252
1	<sup>2</sup> EC	23	113.195	-497.071	0.9991	5.207	72900	0.9959	9.735	16488
2			118.798	-497.180	0.9991	5.208	72893	0.9959	9.742	16467
3			116.924	-495.901	0.9991	5.210	72830	0.9959	9.690	16642

# <sup>2</sup>DCW-modeling

1	<sup>0</sup> EC	8	153.759	-656.597	0.9979	7.818	32303	0.9980	6.893	33635
2			149.916	-635.847	0.9979	7.834	32177	0.9980	6.911	33477
3			153.089	-661.713	0.9979	7.815	32331	0.9980	6.896	33603
1	<sup>1</sup> EC	13	117.526	-448.805	0.9988	5.857	57619	0.9990	4.821	68071
2			119.400	-442.533	0.9988	5.866	57434	0.9990	4.830	67744
3			110.481	-438.225	0.9988	5.871	57332	0.9990	4.825	67868
1	<sup>2</sup> EC	26	115.581	-537.107	0.9992	4.725	88550	0.9970	8.277	22824
2			108.701	-534.546	0.9992	4.735	88180	0.9973	7.965	24661
3			113.946	-534.428	0.9992	4.724	88599	0.9972	8.107	23802

 $^{\ast)}N_{op}$  is number of optimized parameters.

HFG invaraint	CWs on probe 1	CWs on probe 2	CWs on probe 3
Chemical elements, $\mathbf{a}_{\mathbf{k}}$			
Н	0.03124	0.17661	0.02428
С	0.00000	0.00000	0.00000
Extended connectivity			
of first order, ${}^{1}\mathbf{EC}_{\mathbf{k}}$			
0003	2.46163	2.24314	2.78192
0004	0.26443	0.12287	0.32249
0006	2.45652	2.36583	2.74739
0007	0.02004	0.00309	0.00068
0009	3.66781	3.52048	4.09422
0010	1.75035	1.64111	1.89861
0013	3.03027	2.84582	3.30193
0016	4.32879	4.07044	4.71470
(0,1) cycle codes, <b>CC</b>			
C00	7.83707	7.22255	8.19960
C10	4.86283	4.29464	4.78143
C11	2.84091	2.35837	2.51194

**Table 4.** Calculation of the  ${}^{2}DCW(a_{k}, {}^{1}EC_{k})$  for m-xylene.



CW(CC) = CW(C10) = 4.86283

$$CW(CC) + \sum_{k=1}^{n} CW(a_k) + \sum_{k=1}^{n} CW(^{x}EC_k) = 25.10227$$

 $25.20227^{0.5} = 5.01022$ 

No.	a <sub>k</sub>	<sup>1</sup> EC <sub>k</sub>	CW(a <sub>k</sub> )	$CW(^{1}EC_{k})$
1	С	10	0.00000	1.75035
2	С	7	0.00000	0.02004
3	С	10	0.00000	1.75035
4	С	7	0.00000	0.02004
5	С	7	0.00000	0.02004
6	С	7	0.00000	0.02004
7	Н	3	0.03124	2.46163
8	Н	3	0.03124	2.46163
9	Н	3	0.03124	2.46163
10	Н	3	0.03124	2.46163
11	С	6	0.00000	2.45652
12	Н	4	0.03124	0.26443
13	Н	4	0.03124	0.26443
14	Н	4	0.03124	0.26443
15	С	6	0.00000	2.45652
16	Н	4	0.03124	0.26443
17	Н	4	0.03124	0.26443
18	Н	4	0.03124	0.26443

Training set         Solution	No.	Structures	DCW	NBPeynr	NBP <sub>cacl</sub>	NBPeypr - NBPcalc
1         Ethane         3.10664         -88.60000         -83.70767         -4.82333           2         Propane         3.46307         -42.10000         -41.82001         -0.27999           3         2.2-Dimethylpropane         3.72615         -11.7000         -18.24563         -8.74563           4         2.Methylptonane         3.72615         -11.70000         -10.90285         -0.79715           6         n-Butane         3.78610         -0.50000         -3.85733         -3.35733         -3.57533         -3.57533         -3.57533         -3.57533         -3.57533         -3.57533         -3.57533         -3.57533         -3.57533         -3.57533         -3.57533         -0.5753456         -7.05141           8         n-Hexane         4.52521         86.10000         83.20028         3.099732         -0.33411           1         3.40imethylpentane         4.57267         91.80000         107.01907         2.78993           12         3.2-Linruchylpentane         4.77694         112.00000         112.58599         -0.58599           13         3.2-Dimethylpentane         4.77694         118.20000         112.38801         -3.24200           13         -6.44444         -0.770000         51.67185		Training set		capi	cuci	capi cuic
2         Propane         3.46307         -42.10000         -41.82001         -0.27999           3         2.2-Dimethylpropane         3.97418         9.50000         18.24563         -8.74563           4         2-Methylpropane         3.72615         -11.70000         -10.90285         -0.79715           6         P-Butane         3.78610         -0.50000         -3.85753         3.35753           7         3-Methylpentane         4.36096         68.70000         83.0022         4.99998           9         3.3-Dimethylpentane         4.52521         86.10000         83.0022         4.99998           10         3.4Methylpentane         4.52521         86.10000         88.5018         4.91982           12         2.3-Timethylpentane         4.72267         93.50000         88.58018         4.91982           12         2.3-Timethylpentane         4.72957         114.80000         107.01907         7.8093           13         3.4-Dimethylpentane         4.72957         114.80000         107.01907         7.8093           14         2.3.3-Timethylpentane         4.77504         112.50899         -0.55899         -0.55899           13         3.4-Dimethylbeatae         4.97097         133.00000	1	Ethane	3.10664	-88.60000	-83.70767	-4.89233
3         2.2-Dimethylpropane         3.97418         9.50000         18.24663         -8.74563           4         2.Methylpropane         3.72615         -11.70000         -10.90285         -0.79715           5         2.Methylprotane         3.72615         -11.70000         -3.85753         3.35753           3         Methylprotane         4.30901         63.30000         63.70002         4.99998           9         3.3-Dimethylpentane         4.52521         86.10000         83.0028         3.09732           10         2.3-Dimethylpentane         4.52521         86.10000         88.0028         3.99732           11         3.Methylpentane         4.52267         91.80000         88.58018         3.21982           12         3.2-Lithylpentane         4.72267         91.80000         107.01907         2.78093           13         3.2.3-Dimethylpentane         4.72957         114.80000         107.01907         2.78093           13         3.2-Dimethylpentane         4.77694         118.30000         112.58599         5.71401           13         3.5-Lithyl-3-methylpentane         4.92734         140.30000         130.26100         100.3888         2.96112           2.2.3.4         Tetramethylpentane <td>2</td> <td>Propane</td> <td>3.46307</td> <td>-42.10000</td> <td>-41.82001</td> <td>-0.27999</td>	2	Propane	3.46307	-42.10000	-41.82001	-0.27999
4         2-Methylpropane         3.72615         -11.70000         -10.90285         -0.79715           5         2-Methylpropane         3.72615         -11.70000         -10.90285         -0.79715           7         3-Methylpentane         4.30901         63.30000         57.59486         5.70514           8         n-Hexane         4.36996         68.70000         63.70021         499998           9         3.3-Dimethylpentane         4.52211         86.10000         83.8018         3.09732           10         2.3-Dimethylpentane         4.57267         93.50000         88.58018         3.21982           11         3-Methylpentane         4.72957         109.80000         107.01907         2.78093           12         2.3-Trimethylpentane         4.72957         114.80000         107.01907         7.78093           13         3.4-Dimethylpentane         4.72957         114.80000         112.58599         5.71401           13         3.4-Dimethylpentane         4.72957         114.80000         112.58599         5.71401           13         3.4-Dimethylpentane         4.72957         114.80000         112.58599         5.71401           14         2.3.3-Trimethylpentane         4.92545         <	3	2.2-Dimethylpropane	3.97418	9.50000	18.24563	-8.74563
5         2-Methylpropane         3.72615         -11.70000         -10.90285         -0.79715           6         n-Butane         3.78610         -0.5000         -3.85753         3.3573           7         3-Methylpentane         4.30901         63.0000         57.59486         5.70514           8         n-Hexane         4.36096         68.70000         63.70002         4.99998           9.3Dimethylpentane         4.55217         86.10000         83.02688         3.09732           10         2.3-Dimethylpentane         4.57267         91.80000         82.76059         7.03941           13         3-Acthylpentane         4.57267         91.80000         107.01907         7.78093           15         3.3-Dimethylpentane         4.72957         109.80000         107.01907         7.78093           15         3.3-Dimethylpentane         4.72957         114.80000         112.58599         0.58599           16         3-Firthyl-3-methylpentane         4.77694         118.50000         112.58509         3.71401           17         3-thyl-3-methylpentane         4.92545         133.00000         130.25803         3.24200           12         2.2.3-1-Timethylpentane         4.97097         137.50000	4	2-Methylbutane	4.02814	27.80000	24.58701	3.21299
6         n-Butane         3.78610         -0.50000         -3.85753         3.35753           7         3-Methylpentane         4.36090         63.70001         57.9486         5.70514           8         n-Hexane         4.36090         68.70000         83.00268         3.09732           10         2.3-Dimethylpentane         4.52315         88.61000         88.76018         3.09732           10         2.3-Dimethylpentane         4.5215         89.80000         88.58018         3.21982           12         3Dimethylpentane         4.72577         19.80000         88.58018         3.21982           13         2.2,3-Trimethylpentane         4.77694         118.80000         107.01907         2.78093           14         2.3,3-Trimethylpentane         4.77694         118.80000         112.58599         -5.71401           15         3.3-Dimethylpentane         4.92754         140.30000         130.26100         10.03900           12         2.3.3-Trimethylpentane         4.92734         140.30000         130.303882         2.31611           2.2,3.4-Tetramethylpentane         4.92734         122.3000         130.26100         10.03900           12         2.3.3-Trimethylhexane         4.97097         136.	5	2-Methylpropane	3.72615	-11.70000	-10.90285	-0.79715
7         3-Methylpentane         4.30901         63.30000         57.59486         5.70514           8         n-Hexane         4.36096         68.70000         63.70002         4.99998           9         3-Dimethylpentane         4.52515         88.0000         83.00268         3.09732           10         2.3-Dimethylpentane         4.5221         86.10000         83.0268         3.09732           11         3-Methylpentane         4.57267         91.80000         88.58018         4.91982           12         3-Eihylpentane         4.72957         109.80000         107.01907         7.78093           15         3.3-Dimethylpentane         4.72957         114.80000         112.58599         -0.58599           16         3-Eihyl-3-methylpentane         4.77694         118.20000         112.58500         3.24200           17         3-Eihyl-2-methylpentane         4.92734         140.30000         130.03888         2.96112           2.2.3.4-Tetramethylpentane         4.92797         133.00000         130.26100         10.03900           2.2.3.4-Tetramethylpentane         4.97097         136.50000         135.38839         -8.8839           2.2.2.4-Trimethylhexane         4.97097         136.6000         135.18746	6	n-Butane	3.78610	-0.50000	-3.85753	3.35753
8         n-Hexane         4.36096         68.70000         63.70002         4.99998           9         3.3-Dimethylpentane         4.52521         86.10000         83.00268         3.09732           10         2.3-Dimethylpentane         4.52521         88.50000         82.76059         7.039411           11         3-Methylhexane         4.57267         91.80000         88.58018         4.91982           12         3.2-Irimethylpentane         4.72957         110.80000         107.01907         2.78093           13         2.3-Trimethylpentane         4.72957         114.80000         112.58599         -0.58599           16         3-Ethyl-3-methylpentane         4.77604         118.30000         112.35800         3.24200           12         2.3.3-Tertramethylpentane         4.92734         140.30000         130.26100         10.03900           12         2.3.3-Tertramethylpentane         4.92734         122.30000         130.26100         -7.96100           2         2.4.4-Trimethylpentane         4.92734         122.30000         130.26100         -7.96100           2         2.4.4-Trimethylpentane         4.97097         130.60000         133.8839         -8.8839           2         2.4.4-Trimethylpentane </td <td>7</td> <td>3-Methylpentane</td> <td>4.30901</td> <td>63.30000</td> <td>57.59486</td> <td>5.70514</td>	7	3-Methylpentane	4.30901	63.30000	57.59486	5.70514
9         3,3-Dimethylpentane         4.52521         86,1000         83.00268         3.09732           10         2,3-Dimethylpentane         4.52215         89.8000         82.76059         7.03941           11         3-Methylpentane         4.57267         91.80000         88.58018         3.21982           12         3-Eithylpentane         4.57267         93.50000         88.58018         4.91982           13         2,2,3-Trimethylpentane         4.772957         114.80000         107.01907         7.78093           14         2,3-Trimethylpentane         4.77504         112.0000         112.58599         -0.58599           16         3-Eithyl-2-methylpentane         4.27544         118.30000         130.01888         2.96112           12         2,3-3-Trimethylpentane         4.92734         123.30000         130.03888         2.96112           21         2,3-4-Tetramethylpentane         4.97097         137.0000         135.38839         -2.38839           22         2,4-4-Tetramethylpentane         4.97097         136.6000         135.38839         -2.88439           23         2,4-4-Tetramethylpentane         4.97097         136.6000         135.38839         -4.78849           24         2,4-4-Tetramet	8	n-Hexane	4.36096	68.70000	63.70002	4.99998
10         2,3-Dimethylpentane         4.52315         89.80000         82.76059         7.03941           11         3-Methylpextane         4.57267         91.80000         88.58018         3.21982           12         3-Ethylpentane         4.57267         95.50000         88.58018         4.91982           13         2,2,3-Trimethylpentane         4.72957         109.80000         107.01907         2.78093           14         2,3,3-Trimethylpentane         4.77694         112.00000         112.58599         -0.58599           15         3.5.Dimethylbexane         4.77504         115.60000         112.35800         3.24200           18         2.2.Dimethylbentane         4.92734         140.30000         130.26100         10.03900           2.2.3,3-Tertamethylpentane         4.92734         122.30000         130.26100         -7.96100           2.3.3-Trimethylpentane         4.92734         122.30000         133.28839         2.31161           2.2.3,4-Tertamethylpentane         4.92734         122.30000         133.58839         4.78839           2.3.3-Dicthylpentane         5.01606         146.20000         140.68737         5.51263           2.2.4,4-Trimethylpentane         5.01421         140.40000         140.46996	9	3.3-Dimethylpentane	4.52521	86.10000	83.00268	3.09732
11         3-Methylhexane         4.57267         91.80000         88.58018         3.21982           12         3-Eithylpentane         4.57267         93.50000         187.0000         17.01907         2.78093           13         2.3.3-Trimethylpentane         4.722957         114.80000         107.01907         2.78093           14         2.3.3-Trimethylpentane         4.77694         118.30000         112.58599         -0.58599           16         3-Ethyl-3-methylpentane         4.77500         115.60000         112.35890         5.71401           17         3-Ethyl-2-methylpentane         4.92545         133.0000         130.03888         2.96112           12         2.3.3-Trimethylpentane         4.92545         133.0000         130.03888         2.96112           12         2.3.3-Trimethylpentane         4.92734         142.30000         130.28839         2.31161           22         2.4.4-Trimethylpentane         4.97097         136.60000         133.8839         4.8839           25         3.3-Diethylpentane         5.01606         146.20000         140.68737         5.51263           2         2.4-4-Trimethylhexane         5.01421         140.40000         140.46996         -0.06996           2	10	2.3-Dimethylpentane	4.52315	89.80000	82.76059	7.03941
12         3-Ethylpentane         4.57267         93.50000         88.58018         4.91982           13         2,2,3-Tirmethylpentane         4.72957         114,80000         107.01907         7.78093           15         3,3-Dimethylpentane         4.77694         112.00000         112.58599         -0.58599           16         3-Ethyl-3-methylpentane         4.77694         118.30000         112.58509         5.71401           17         3-Ethyl-3-methylpentane         4.77590         115.60000         112.58509         5.71401           17         3-Ethyl-2-methylpentane         4.92734         140.30000         130.26100         10.03900           2,2,3,4-Tetramethylpentane         4.92734         122.30000         130.26100         -7.96100           2,2,4,4-Tetramethylpentane         4.97097         135.5000         135.38839         2.88839           2,3,2-Tirmethylhexane         4.97097         136.60000         135.38839         -8.88839           2,3,3-Tirmethylpentane         5.01606         146.20000         140.68737         5.51263           2,4,4-Tirmethylhexane         5.01421         143.30000         140.46996         -0.60996           2,4,4-Tirmethylhexane         5.01421         133.80000         140.46996	11	3-Methylhexane	4.57267	91.80000	88.58018	3.21982
13         22.3-Trimethylpentane         4.72957         109.80000         107.01907         2.78093           14         2.3.3-Trimethylpentane         4.72957         114.80000         107.01907         7.78093           15         3.3-Dimethylbexane         4.77694         112.00000         112.58599         -0.58599           16         3-Eithyl-3-methylpentane         4.77504         112.00000         112.58599         5.71401           17         3-Eithyl-2-methylpentane         4.25861         49.70000         51.67185         -1.97185           19         2.2,3.4-Tetramethylpentane         4.925345         133.00000         130.26100         -7.96100           21         2.3.3-Trimethylhexane         4.97097         137.70000         135.38839         2.31161           22         2.4.4-Tetramethylpentane         4.97097         136.0000         135.38839         -8.88839           24         2.4.4-Trimethylhexane         4.97097         136.70000         135.16746         1.53254           23         3-Diethylpentane         5.01606         146.20000         140.46996         -0.06996           2.4-dimethyl-3-ethylhexane         5.01421         133.80000         140.46996         -6.66996           2.4-Ethyl-4-methylhexane<	12	3-Ethylpentane	4 57267	93 50000	88 58018	4 91982
14         2.3.3-Trimethylpentane         4.72957         114.80000         107.01907         7.78093           15         3.3-Dimethylpentane         4.77694         118.00000         112.88599         -0.58599           16         3-Eithyl-3-methylpentane         4.77504         118.30000         112.35800         3.24200           17         3-Eithyl-2-methylpentane         4.27544         115.6000         112.35800         3.24200           18         2.2-Dimethylpentane         4.92734         140.30000         130.03888         2.96112           21         2.3.3-Tertamethylpentane         4.92734         123.00000         130.03888         2.96112           21         2.3.4-Tertamethylpentane         4.97097         126.50000         135.38839         2.31161           22         2.2.4.4-Tertamethylpentane         4.97097         126.50000         135.38839         4.88839           23.3-Diethylpentane         5.01606         146.20000         140.68737         5.51263           26         2.4-dimethyl-3-ethylpentane         5.01421         133.80000         140.46996         -6.66996           29         2-Methyloctane         5.015892         141.20000         145.72428         -4.242428           21         3.25-D	13	2 2 3-Trimethylpentane	4 72957	109 80000	107 01907	2 78093
15         3.3-Dimethylhexane         4.77694         112.0000         112.58599         -0.58599           16         3-Ethyl-3-methylpentane         4.77694         118.30000         112.58599         5.71401           17         3-Ethyl-2-methylpentane         4.77500         115.60000         112.35800         3.24200           18         2.2-Dimethylbutane         4.25861         49.7000         51.67185         -1.97185           19         2.2.3.3-Tetramethylpentane         4.92734         140.30000         130.03888         2.96112           21         2.3.3-Trimethylhexane         4.97097         137.70000         135.38839         2.31161           22         2.2.4.4-Trimethylhexane         4.97097         136.0000         135.38839         2.8839           23         3.2.4.4-Trimethylhexane         4.97097         136.0000         135.38839         4.78839           25         3.3-Diethylpentane         5.01401         140.40000         140.68737         5.51263           26         2.4-dimethyl-3-ethylpentane         5.01421         133.30000         145.72428         -4.24248           23         3-Methyloctane         5.05892         144.20000         145.72428         -1.52428           2.4-Ethyl-4-methylhex	14	2 3 3-Trimethylpentane	4 72957	114 80000	107 01907	7 78093
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	15	3.3-Dimethylhexane	4.77694	112.00000	112.58599	-0.58599
173-Ethyl-2-methylpentane4.77500115.60000112.358003.24200182.2-Dimethylbutane4.2586149.7000051.67185 $-1.97185$ 192.2,3.3-Tetramethylpentane4.92545133.0000130.2610010.03900202.2,3.4-Tetramethylpentane4.92545133.0000130.288392.31161212.3.3-Trimethylhexane4.97097137.70000135.388392.31161222.2,4.4-Tetramethylpentane4.97097126.50000135.38839-8.88839242.4.4-Trimethylhexane4.97097130.60000135.38839-8.78839253.3-Diethylpentane4.96909136.70000135.167461.53254273-Ethyl-2-methylhexane5.01421140.40000140.68976-0.06996284-Ethyl-2-methylhexane5.01421133.30000140.46996-0.06996292-Methyloctane5.05892144.20000145.72428-2.242428303-Methyloctane5.05892144.20000145.72428-4.52428314-Ethylheptane5.01421136.00000140.46996-4.46996322,2-Dimethylheptane5.01421136.0000140.46996-4.46996333,5-Dimethylheptane5.01421136.0000140.46996-4.46996342,6-Dimethylheptane5.01421136.0000140.46996-4.46996353,5-Dimethylheptane5.01421136.0000140.46996-4.46996342,6-Dimethylheptane<	16	3-Ethyl-3-methylpentane	4.77694	118.30000	112.58599	5.71401
18         2,2-Dimethylbutane         4.25861         49,7000         51.67185         -1.97185           19         2,2,3,3-Tertarmethylpentane         4.92734         140.30000         130.26100         10.03900           20         2,2,3,4-Tetramethylpentane         4.92734         140.30000         130.26100         -7.96100           21         2,3,3-Trimethylhexane         4.97097         137.70000         135.38839         2.31161           22         2,2,4,4-Trimethylhexane         4.97097         126.50000         135.38839         4.88839           23         2,2,4-Trimethylhexane         4.97097         126.50000         135.38839         4.78839           25         3,3-Diethylpentane         5.01606         146.20000         140.68737         5.51263           26         2,4-dimethyl-3-ethylpentane         5.01421         140.40000         140.46996         -6.66996           28         4-Ethyl-2-methylhexane         5.01421         143.30000         145.72428         -1.52428           30         3-Methyloctane         5.05892         143.30000         145.72428         -4.52428           32         2,2-Dimethylheptane         5.01421         135.20000         140.68996         -4.6996           31	17	3-Ethyl-2-methylpentane	4 77500	115 60000	112.35800	3 24200
19         2,2,3,3-Tetramethylpentane         4.92734         140.30000         130.26100         10.03900           20         2,2,3,3-Tetramethylpentane         4.92734         140.30000         130.03888         2.96112           21         2,3,3-Titimethylhexane         4.97097         137.70000         135.38839         2.31161           22         2,2,4-Titimethylhexane         4.97097         126.50000         135.38839         -8.88839           24         2,4,4-Trimethylhexane         4.97097         130.60000         135.38839         -4.78839           25         3,3-Diethylpentane         5.01606         146.20000         140.68737         5.51263           26         2,4-dimethyl-3-ethylpentane         5.01421         140.40000         140.46996         -0.06996           28         4-Ethyl-2-methylhexane         5.01421         133.8000         145.72428         -1.52428           29         2-Methyloctane         5.05892         144.20000         145.72428         -4.52428           31         4-Ethylheptane         5.01421         135.0000         140.46996         -5.26996           31         2,5-Dimethylheptane         5.01421         135.0000         140.46996         -5.26996           31	18	2 2-Dimethylbutane	4 25861	49 70000	51 67185	-1 97185
10         10         10         10         100         130.0000         130.03888         2.96012           21         2,3,3-Trimethylhexane         4.97097         137.70000         135.38839         2.31161           22         2,2,4,4-Tetramethylpentane         4.92734         122.30000         130.03888         2.96112           23         2,2,4-Trimethylhexane         4.97097         130.60000         135.38839         -7.96100           23         2,2,4-Trimethylhexane         4.97097         130.60000         135.38839         -4.78839           24         2,4-4-Trimethylhexane         5.01606         146.20000         140.68973         5.51263           26         2,4-dimethyl-3-ethylpentane         5.01421         133.80000         140.46996         -0.06996           27         3-Ethyl-4-methylhexane         5.01421         133.80000         140.46996         -0.06996           28         4-Ethyl-2-methylhexane         5.05892         143.20000         145.72428         -1.52428           21         4-Ethylheptane         5.015892         141.20000         145.72428         -1.52428           32         2,2-Dimethylheptane         5.01421         136.00000         140.46996         -5.26996	19	2 2 3 3-Tetramethylpentane	4 92734	140 30000	130 26100	10.03900
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	20	2 2 3 4-Tetramethylpentane	4 92545	133,00000	130.03888	2.96112
212222,2,4,4-Tetramethylpentane4.92734122.30000130.26100-7.96100232,2,4-Trimethylhexane4.97097126.50000135.38839-8.88839242,4,4-Trimethylhexane4.97097130.60000135.38839-4.78839253,3-Diethylpentane5.01606146.20000140.687375.51263262,4-dirmethyl-3-ethylpentane5.01421140.40000140.46996-0.06996262,4-dirmethyl-2-ethylpentane5.01421133.80000140.46996-6.66996273-Ethyl-4-methylhexane5.01421133.80000140.72428-2.42428303-Methyloctane5.05892141.20000145.72428-1.52428314-Ethylheptane5.01506132.70000140.68737-7.98737332,5-Dimethylheptane5.01421136.00000140.46996-4.46996353,5-Dimethylheptane5.01421136.00000140.46996-4.46996363-Methyl-3-ethylhexane5.01606110.60000140.68737-0.0873737Benzene4.4654680.1000075.80864.1191448Toluene4.74556110.60000140.00105-0.9010540p-Xylene5.01022139.10000140.00105-0.90105411-Methyl-3-ethylbenzene5.18892161.30000140.00105-0.90105421-Methyl-4-ethylbenzene5.36168183.80000181.304632.49537431,3,5-Trimethylbenzene <td>21</td> <td>2 3 3-Trimethylhexane</td> <td>4 97097</td> <td>137 70000</td> <td>135 38839</td> <td>2.31161</td>	21	2 3 3-Trimethylhexane	4 97097	137 70000	135 38839	2.31161
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	22	2.2.4.4-Tetramethylpentane	4 92734	122,30000	130 26100	-7 96100
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	22	2.2.4.Trimethylbeyane	4 97097	126 50000	135 38839	-8 88839
25       3,3-Diethylpentane       5.01606       146.2000       140.68737       5.51263         26       2,4-dimethyl-3-ethylpentane       4.96909       136.70000       135.16746       1.53254         27       3-Ethyl-4-methylhexane       5.01421       140.40000       140.46996       -0.06996         28       4-Ethyl-2-methylhexane       5.01421       133.80000       145.72428       -2.42428         30       3-Methyloctane       5.05892       144.20000       145.72428       -1.52428         31       4-Ethyl-heptane       5.01606       132.70000       145.72428       -4.52428         32       2,2-Dimethylheptane       5.01606       132.70000       140.68737       -7.98737         33       2,5-Dimethylheptane       5.01421       136.00000       140.46996       -4.46996         34       2,6-Dimethylheptane       5.01421       136.00000       140.46996       -4.46996         36       3-Methyl-3-ethylhexane       5.01606       140.60000       140.68737       -0.08737         37       Benzene       4.46546       80.10000       75.98086       4.11914         38       Toluene       4.74566       110.60000       140.00105       -0.90105         41	23	2 4 4-Trimethylhexane	4 97097	130,60000	135 38839	-4 78839
25         District         District         District         District           26         2.4-dimethyl-3-ethylpentane         4.96909         136.70000         135.16746         1.53254           27         3-Ethyl-4-methylhexane         5.01421         140.40000         140.46996         -0.06996           28         4-Ethyl-2-methylhexane         5.01421         133.80000         145.72428         -2.42428           30         3-Methyloctane         5.05892         144.20000         145.72428         -1.52428           31         4-Ethylheptane         5.05892         141.20000         145.72428         -4.52428           32         2,2-Dimethylheptane         5.01606         132.70000         140.68737         -7.98737           33         2,5-Dimethylheptane         5.01421         136.00000         140.46996         -4.46996           34         2,6-Dimethylheptane         5.01421         136.00000         140.46996         -5.26996           35         3,5-Dimethylheptane         5.01421         136.00000         140.68737         -0.08737           37         Benzene         4.46546         80.10000         75.98086         4.11914           38         Toluene         5.01022         138.40000 <td>25</td> <td>3 3-Diethylpentane</td> <td>5.01606</td> <td>146 20000</td> <td>140 68737</td> <td>5 51263</td>	25	3 3-Diethylpentane	5.01606	146 20000	140 68737	5 51263
20       2,4-unitedry 5-curyptimize       4,5050       135,10000       140,46996       -0.06996         27       3.Ethyl-4-methylhexane       5.01421       133,80000       140,46996       -0.06996         28       4-Ethyl-2-methylhexane       5.01421       133,80000       145,72428       -2.42428         30       3-Methyloctane       5.05892       144,20000       145,72428       -1.52428         31       4-Ethylheptane       5.01606       132,70000       140,68737       -7.98737         33       2,5-Dimethylheptane       5.01421       135,00000       140,46996       -4.46996         34       2,6-Dimethylheptane       5.01421       135,00000       140,46996       -4.46996         35       3,5-Dimethylheptane       5.01421       136,00000       140,46996       -4.46996         36       3-Methyl-3-ethylhexane       5.01606       140,60000       140,46996       -4.46996         36       3-Methyl-3-ethylhexane       5.01002       139,10000       140,0105       -0.008737         37       Benzene       4.74566       110,60000       140,00105       -0.00105         40       p-Xylene       5.01022       139,10000       140,00105       -1.60105         41	25	2 <i>A</i> -dimethyl_3-ethylpentane	1 96909	136 70000	135 16746	1 53254
21       35.1421       140.40000       140.46996       -6.66996         28       4-Ethyl-2-methylhexane       5.05892       143.30000       145.72428       -2.42428         30       3-Methyloctane       5.05892       144.20000       145.72428       -1.52428         31       4-Ethyl-Iphptane       5.05892       141.20000       145.72428       -4.52428         32       2,2-Dimethylheptane       5.01606       132.70000       140.68977       -7.98737         33       2,5-Dimethylheptane       5.01421       136.00000       140.46996       -4.6996         34       2,6-Dimethylheptane       5.01421       136.00000       140.46996       -5.26996         35       3,5-Dimethylheptane       5.01421       136.00000       140.46996       -4.46996         36       3-Methyl-3-ethylhexane       5.01606       140.60000       140.68737       -0.08737         37       Benzene       4.46546       80.10000       140.68737       -0.08737         37       Benzene       5.01022       138.40000       140.00105       -0.90105         40       p-Xylene       5.01022       138.40000       140.00105       -1.60105         41       1-Methyl-4-ethylbenzene       5.18	20	3-Ethyl-1-methylbeyane	5.01/21	140 40000	1/0/46996	-0.06096
29       2-Methyloctane       5.05421       19530000       145.72428       -2.42428         30       3-Methyloctane       5.05892       144.20000       145.72428       -2.42428         31       4-Ethylheptane       5.05892       141.20000       145.72428       -4.52428         32       2,2-Dimethylheptane       5.01606       132.70000       140.68737       -7.98737         33       2,5-Dimethylheptane       5.01421       136.00000       140.46996       -4.46996         34       2,6-Dimethylheptane       5.01421       136.00000       140.46996       -5.26996         35       3,5-Dimethylheptane       5.01606       104.06000       140.66996       -4.46996         36       3-Methyl-3-ethylhexane       5.01000       140.46996       -4.46996         36       3-Methyl-3-ethylhexane       5.01022       138.40000       140.00105       -0.90105         40       p-Xylene       5.01022       138.40000       140.00105       -0.90105         41       1-Methyl-3-ethylbenzene       5.18892       161.30000       161.00188       0.29812         42       1-Methyl-4-ethylbenzene       5.26149       164.70000       169.53030       -4.83030         44       1,2,3,4-	27	4-Ethyl-2-methylhexane	5.01421	133 80000	140.46996	-6.66996
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	20	2-Methyloctane	5.05892	143 30000	145 72428	-0.00770
31         4-Ethylketane         5.05092         141.20000         145.72428         -4.52428           31         4-Ethylketane         5.05892         141.20000         145.72428         -4.52428           32         2,2-Dimethylkeptane         5.01606         132.7000         140.68737         -7.98737           33         2,5-Dimethylkeptane         5.01421         136.00000         140.46996         -4.46996           34         2,6-Dimethylkeptane         5.01421         135.20000         140.46996         -4.46996           35         3,5-Dimethylkeptane         5.01606         140.60000         140.46996         -4.46996           36         3-Methyl-3-ethylkexane         5.01606         140.60000         140.68737         -0.08737           37         Benzene         4.46546         80.10000         75.98086         4.11914           38         Toluene         5.01022         139.10000         140.00105         -0.90105           40         p-Xylene         5.01022         138.40000         140.00105         -1.60105           41         1-Methyl-a-ethylbenzene         5.1892         161.30000         161.00188         0.29812           42         1-Methyl-4-ethylbenzene         5.26149	30	3-Methyloctane	5.05892	144 20000	145 72428	-1 52428
32       2,2-Dimethylheptane       5.01606       132.70000       140.68737       -7.98737         33       2,5-Dimethylheptane       5.01421       136.00000       140.46996       -4.46996         34       2,6-Dimethylheptane       5.01421       135.20000       140.46996       -4.46996         35       3,5-Dimethylheptane       5.01421       136.00000       140.46996       -4.46996         36       3-Methyl-3-ethylhexane       5.01606       140.60000       140.68737       -0.08737         37       Benzene       4.46546       80.10000       75.98086       4.11914         38       Toluene       5.01022       139.10000       140.00105       -0.90105         40       p-Xylene       5.01022       138.40000       140.00105       -0.90105         41       1-Methyl-3-ethylbenzene       5.18892       161.30000       161.00188       0.29812         42       1-Methyl-4-ethylbenzene       5.26149       164.70000       169.53030       -4.83030         44       1,2,3,4-Tetramethylbenzene       5.36168       181.10000       181.30463       2.49537         45       1,3-Diethylbenzene       5.36168       183.80000       181.30463       2.49537         47	31	4-Ethylhentane	5.05892	141 20000	145 72428	-4 52428
33       2,2-Dincthylheptate       5.01000       140.0000       140.46996       -4.46996         34       2,6-Dimethylheptate       5.01421       136.00000       140.46996       -5.26996         35       3,5-Dimethylheptate       5.01421       135.20000       140.46996       -5.26996         36       3-Methyl-3-ethylhexane       5.01606       140.60000       140.46996       -4.46996         36       3-Methyl-3-ethylhexane       5.01606       140.60000       140.68737       -0.08737         37       Benzene       4.46546       80.10000       75.98086       4.11914         38       Toluene       5.01022       139.10000       140.00105       -0.90105         40       p-Xylene       5.01022       138.40000       140.00105       -0.90105         41       1-Methyl-3-ethylbenzene       5.18892       161.30000       161.00188       0.29812         42       1-Methyl-4-ethylbenzene       5.26149       164.70000       169.53030       -4.83030         44       1,2,3,4-Tetramethylbenzene       5.50129       205.00000       197.71160       7.28840         45       1,3-Diethylbenzene       5.36168       181.10000       181.30463       2.49537         47	32	2 2-Dimethylhentane	5.03092	132 70000	140 68737	-7 98737
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	33	2 5-Dimethylheptane	5 01421	136,00000	140 46996	-4 46996
352,0-Dimethylheptane5,01421135,20000140,46996-4,46996363,5-Dimethylheptane5,01606140,60000140,68737-0.0873737Benzene4,4654680,1000075,980864,1191438Toluene4,74566110,60000108,909961.6900439m-Xylene5,01022139,10000140,00105-0.9010540p-Xylene5,01022138,40000140,00105-1.60105411-Methyl-3-ethylbenzene5,18892161,30000161,001880.29812421-Methyl-4-ethylbenzene5,26149164,70000169,53030-4.83030441,2,3,4-Tetramethylbenzene5,36168181,10000181,30463-0.20463451,3-Diethylbenzene5,36168183,80000181,304632.49537471-Methyl-4-n-propylbenzene5,43194193,90000189,56159-3.16675481,2-Dimethyl-3-ethylbenzene5,43194193,90000189,56159-1.16159501,3-Dimethyl-4-ethylbenzene5,50129196,80000189,56159-1.16159511,2,4,5-Tetramethylbenzene5,50129196,80000189,56159-5,76159511,2,4,5-Tetramethylbezene5,50129196,80000197,71160-0.9116052Naphthalene5,68346218,00000271,96661-1.9666154Acenaphtylene6,13314270,00000271,96661-1.9666154Acenaphtylene6,13314270,0000	34	2.6-Dimethylheptane	5.01421	135 20000	140.46996	-5 26996
363.93.91.90.00001.40.407004.40570363-Methyl-3-ethylhexane5.01606140.60000140.68737-0.0873737Benzene4.4654680.1000075.980864.1191438Toluene4.74566110.60000108.909961.6900439m-Xylene5.01022139.10000140.00105-0.9010540p-Xylene5.01022138.40000140.00105-1.60105411-Methyl-3-ethylbenzene5.18892161.30000161.001880.29812421-Methyl-4-ethylbenzene5.26149164.70000169.53030-4.83030441,2,3,4-Tetramethylbenzene5.36168181.10000181.30463-0.20463451,3-Diethylbenzene5.36168183.80000181.304632.49537471-Methyl-4-n-propylbenzene5.43194193.90000189.561594.33841491,3-Dimethyl-3-ethylbenzene5.43194183.80000189.56159-1.16159501,3-Dimethyl-5-ethylbenzene5.43194183.80000189.56159-1.16159511,2,4,5-Tetramethylbenzene5.43194183.80000189.56159-5.76159511,2,4,5-Tetramethylbenzene5.68346218.00000271.96661-1.9666152Naphthalene5.68346218.00000271.96661-1.9666154Acenaphthylene6.10314270.00000271.96661-1.96661	35	3 5-Dimethylheptane	5.01421	136,00000	140.46996	-4 46996
3034.0000140.0000140.0000140.0000140.000037Benzene4.4654680.1000075.980864.1191438Toluene4.74566110.60000108.909961.6900439m-Xylene5.01022139.10000140.00105-0.9010540p-Xylene5.01022138.40000140.00105-0.90105411-Methyl-3-ethylbenzene5.18892161.30000161.001880.29812421-Methyl-4-ethylbenzene5.18892162.00000161.001880.99812431,3,5-Trimethylbenzene5.26149164.70000169.53030-4.83030441,2,3,4-Tetramethylbenzene5.30129205.00000197.711607.28840451,3-Diethylbenzene5.36168181.10000181.304632.49537461,4-Diethylbenzene5.36168183.80000186.96675-3.16675481,2-Dimethyl-3-ethylbenzene5.43194193.90000189.561594.33841491,3-Dimethyl-4-ethylbenzene5.43194183.80000189.56159-1.16159501,3-Dimethyl-5-ethylbenzene5.43194183.80000189.56159-5.76159511,2,4,5-Tetramethylbezene5.50129196.80000197.71160-0.9116052Naphthalene5.68346218.00000271.96661-1.9666154Acenaphthylene6.13314270.00000271.96661-1.96661	36	3-Methyl_3-ethylbevane	5.01421	140 60000	140.40770	-0.08737
57Defizence4.7634600.1000012.90004.1191438Toluene4.74566110.60000108.909961.6900439m-Xylene5.01022139.10000140.00105-0.9010540p-Xylene5.01022138.40000140.00105-1.60105411-Methyl-3-ethylbenzene5.18892161.30000161.001880.29812421-Methyl-4-ethylbenzene5.26149164.70000169.53030-4.83030431,3,5-Trimethylbenzene5.26149164.70000169.53030-4.83030441,2,3,4-Tetramethylbenzene5.50129205.00000197.711607.28840451,3-Diethylbenzene5.36168181.10000181.30463-0.20463461,4-Diethylbenzene5.36168183.80000186.96675-3.16675481,2-Dimethyl-3-ethylbenzene5.43194193.90000189.561594.33841491,3-Dimethyl-4-ethylbenzene5.43194188.40000189.56159-1.16159501,3-Dimethyl-5-ethylbenzene5.43194183.80000189.56159-5.76159511,2,4,5-Tetramethylbezene5.50129196.80000197.71160-0.9116052Naphthalene5.68346218.00000271.96661-1.9666154Acanaphthylene6.13314270.00000271.96661-1.9666154Acanaphthylene6.13314270.00000271.96661-1.96661	37	Benzene	4 46546	80 10000	75 98086	4 11914
30101.00000100.0000100.00001.0000039m-Xylene5.01022139.10000140.00105-0.9010540p-Xylene5.01022138.40000140.00105-1.60105411-Methyl-3-ethylbenzene5.18892161.30000161.001880.29812421-Methyl-4-ethylbenzene5.18892162.00000161.001880.99812431,3,5-Trimethylbenzene5.26149164.70000169.53030-4.83030441,2,3,4-Tetramethylbenzene5.50129205.00000197.711607.28840451,3-Diethylbenzene5.36168181.10000181.30463-0.20463461,4-Diethylbenzene5.36168183.80000181.304632.49537471-Methyl-4-n-propylbenzene5.40986183.80000189.561594.33841491,3-Dimethyl-3-ethylbenzene5.43194193.90000189.561594.33841491,3-Dimethyl-5-ethylbenzene5.50129196.80000197.71160-0.91160501,3-Dimethyl-5-ethylbenzene5.50129196.80000197.71160-0.91160511,2,4,5-Tetramethylbezene5.50129196.80000197.7160-0.9116052Naphthalene5.68346218.00000271.96661-1.9666154Acenaphthylene6.13314270.00000271.96661-1.96661	38	Toluene	4 74566	110 60000	108 90996	1 69004
35In-Kylenc5.01022135.10000140.00105-0.0010540p-Xylene5.01022138.40000140.00105-1.60105411-Methyl-3-ethylbenzene5.18892161.30000161.001880.29812421-Methyl-4-ethylbenzene5.18892162.00000161.001880.99812431,3,5-Trimethylbenzene5.26149164.70000169.53030-4.83030441,2,3,4-Tetramethylbenzene5.50129205.00000197.711607.28840451,3-Diethylbenzene5.36168181.10000181.30463-0.20463461,4-Diethylbenzene5.36168183.80000181.304632.49537471-Methyl-4-n-propylbenzene5.40986183.80000186.96675-3.16675481,2-Dimethyl-3-ethylbenzene5.43194193.90000189.561594.33841491,3-Dimethyl-4-ethylbenzene5.43194188.40000189.56159-1.16159501,3-Dimethyl-5-ethylbenzene5.43194183.80000189.56159-5.76159511,2,4,5-Tetramethylbezene5.68346218.00000219.12022-1.1202253Acenaphthylene6.13314270.00000271.96661-1.96661544.00000271.96661-1.96661-1.96661	39	m-Xylene	5.01022	139 10000	140.00105	-0.90105
40PAytene5.01022136.40000140.00103140.00103411-Methyl-3-ethylbenzene5.18892161.30000161.001880.29812421-Methyl-4-ethylbenzene5.18892162.00000161.001880.99812431,3,5-Trimethylbenzene5.26149164.70000169.53030-4.83030441,2,3,4-Tetramethylbenzene5.50129205.00000197.711607.28840451,3-Diethylbenzene5.36168181.10000181.30463-0.20463461,4-Diethylbenzene5.36168183.80000181.304632.49537471-Methyl-4-n-propylbenzene5.40986183.80000186.96675-3.16675481,2-Dimethyl-3-ethylbenzene5.43194193.90000189.561594.33841491,3-Dimethyl-4-ethylbenzene5.43194188.40000189.56159-1.16159501,3-Dimethyl-5-ethylbenzene5.50129196.80000197.71160-0.9116052Naphthalene5.68346218.00000219.12022-1.1202253Acenaphthylene6.13314270.00000271.96661-1.96661544.00000271.96661-1.96661-1.96661-1.96661	40	n-Xylene	5.01022	138 40000	140.00105	-0.90105
411-Methyl-9-chrybolizete5.18892161.30000161.301880.23612421-Methyl-4-ethylbenzene5.18892162.00000161.001880.99812431,3,5-Trimethylbenzene5.26149164.70000169.53030-4.83030441,2,3,4-Tetramethylbenzene5.50129205.00000197.711607.28840451,3-Diethylbenzene5.36168181.10000181.30463-0.20463461,4-Diethylbenzene5.36168183.80000181.304632.49537471-Methyl-4-n-propylbenzene5.40986183.80000186.96675-3.16675481,2-Dimethyl-3-ethylbenzene5.43194193.90000189.561594.33841491,3-Dimethyl-4-ethylbenzene5.43194188.40000189.56159-1.16159501,3-Dimethyl-5-ethylbenzene5.50129196.80000197.71160-0.9116052Naphthalene5.68346218.00000219.12022-1.1202253Acenaphthylene6.13314270.00000271.96661-1.96661544.00000271.96661-1.96661-1.96661	40	1-Methyl-3-ethylbenzene	5 18892	161 30000	161 00188	0.29812
421-Methyl-4-ethylochizete5.18892102.00000101.001880.79812431,3,5-Trimethylbenzene5.26149164.70000169.53030-4.83030441,2,3,4-Tetramethylbenzene5.50129205.00000197.711607.28840451,3-Diethylbenzene5.36168181.10000181.30463-0.20463461,4-Diethylbenzene5.36168183.80000181.304632.49537471-Methyl-4-n-propylbenzene5.40986183.80000186.96675-3.16675481,2-Dimethyl-3-ethylbenzene5.43194193.90000189.561594.33841491,3-Dimethyl-4-ethylbenzene5.43194188.40000189.56159-1.16159501,3-Dimethyl-5-ethylbenzene5.43194183.80000189.56159-5.76159511,2,4,5-Tetramethylbezene5.50129196.80000197.71160-0.9116052Naphthalene5.68346218.00000219.12022-1.1202253Acenaphthylene6.13314270.00000271.96661-1.96661544.00000271.96661-1.96661-1.96661	41	1-Methyl-4-ethylbenzene	5 18892	162,00000	161.00188	0.29812
451,3,5-1111111111111111111111111111111111	13	1 3 5-Trimethylbenzene	5 261/19	164 70000	169 53030	-1 83030
441,2,3,41000131,3000131,3000131,3000451,3-Diethylbenzene5.36168181,10000181,30463-0.20463461,4-Diethylbenzene5.36168183,80000181,304632.49537471-Methyl-4-n-propylbenzene5.40986183,80000186,96675-3.16675481,2-Dimethyl-3-ethylbenzene5.43194193,90000189,561594.33841491,3-Dimethyl-4-ethylbenzene5.43194188,40000189,56159-1.16159501,3-Dimethyl-5-ethylbenzene5.43194183,80000189,56159-5.76159511,2,4,5-Tetramethylbezene5.50129196,80000197,71160-0.9116052Naphthalene5.68346218,00000219,12022-1.1202253Acenaphthylene6.13314270,00000271,96661-1.9666154Acenaphthylene6.10516270,00000268,6784010,22160	43	1,2,3,4-Tetramethylbenzene	5 50129	205.00000	197 71160	7 28840
461,4-Diethylbenzene5.36168181.10000181.304632.49537471-Methyl-4-n-propylbenzene5.40986183.80000186.96675-3.16675481,2-Dimethyl-3-ethylbenzene5.43194193.90000189.561594.33841491,3-Dimethyl-4-ethylbenzene5.43194188.40000189.56159-1.16159501,3-Dimethyl-5-ethylbenzene5.43194188.40000189.56159-5.76159511,2,4,5-Tetramethylbezene5.50129196.80000197.71160-0.9116052Naphthalene5.68346218.00000219.12022-1.1202253Acenaphthylene6.13314270.00000271.96661-1.96661	45	1 3-Diethylbenzene	5 36168	181 10000	181 30/63	-0.20040
471-Methyl-4-n-propylbenzene5.50106185.80000181.904032.49537471-Methyl-4-n-propylbenzene5.40986183.80000186.96675-3.16675481,2-Dimethyl-3-ethylbenzene5.43194193.90000189.561594.33841491,3-Dimethyl-4-ethylbenzene5.43194188.40000189.56159-1.16159501,3-Dimethyl-5-ethylbenzene5.43194183.80000189.56159-5.76159511,2,4,5-Tetramethylbezene5.50129196.80000197.71160-0.9116052Naphthalene5.68346218.00000219.12022-1.1202253Acenaphthylene6.13314270.00000271.96661-1.9666154Acenaphthylene6.10516270.00000268.6784010.22160	45	1 4-Diethylbenzene	5 36168	183 80000	181 30/63	2 40537
48       1,2-Dimethyl-3-ethylbenzene       5.43194       193.90000       189.56159       4.33841         49       1,3-Dimethyl-4-ethylbenzene       5.43194       188.40000       189.56159       -1.16159         50       1,3-Dimethyl-5-ethylbenzene       5.43194       188.40000       189.56159       -5.76159         51       1,2,4,5-Tetramethylbezene       5.68346       218.00000       197.71160       -0.91160         52       Naphthalene       5.68346       218.00000       271.96661       -1.96661         54       Accnaphthylene       6.13314       270.00000       271.96661       -1.96661	17	1-Methyl_4_n_nronylbanzana	5.30108	183.80000	186 96675	_3 16675
49       1,3-Dimethyl-4-ethylbenzene       5.43194       195.90000       189.50159       4.53641         49       1,3-Dimethyl-4-ethylbenzene       5.43194       188.40000       189.56159       -1.16159         50       1,3-Dimethyl-5-ethylbenzene       5.43194       183.80000       189.56159       -5.76159         51       1,2,4,5-Tetramethylbezene       5.50129       196.80000       197.71160       -0.91160         52       Naphthalene       5.68346       218.00000       219.12022       -1.12022         53       Acenaphthylene       6.13314       270.00000       271.96661       -1.96661	/19	1 2_Dimethyl_3_ethylbonzone	5 / 210/	103.00000	180.50075	/ 328/1
47       135-Dimethyl-4-ethylotizete       5.43194       186.40000       189.50139       -1.10139         50       1,3-Dimethyl-5-ethylbenzene       5.43194       183.80000       189.56159       -5.76159         51       1,2,4,5-Tetramethylbezene       5.50129       196.80000       197.71160       -0.91160         52       Naphthalene       5.68346       218.00000       219.12022       -1.12022         53       Acenaphthylene       6.13314       270.00000       271.96661       -1.96661	40	1.2-Dimethyl-3-ethylbenzene	5 / 210/	188 /0000	189.50159	-1 16150
50       1,5-Dimethylo-chrybelizene       5.43194       185.00000       189.30139       -5.76159         51       1,2,4,5-Tetramethylbezene       5.50129       196.80000       197.71160       -0.91160         52       Naphthalene       5.68346       218.00000       219.12022       -1.12022         53       Acenaphthylene       6.13314       270.00000       271.96661       -1.96661         54       Acenaphthylene       6.10516       270.00000       268.67840       10.22160	+7 50	1.3 Dimethyl 5 othylbonzona	5 /210/	182 20000	180 56150	5 76150
51       1,2,4,5-1 chainethyloczene       5.50129       196.50000       197.71100       -0.91160         52       Naphthalene       5.68346       218.00000       219.12022       -1.12022         53       Acenaphthylene       6.13314       270.00000       271.96661       -1.96661         54       Acenaphthylene       6.10516       270.00000       268.67840       10.22160	50	1,3-Diffetingi-3-etilyildenzene	5 50120	105.00000	107.30139	-3./0139
52         Reprintation         5.06540         218.00000         219.12022         -1.12022           53         Acenaphthylene         6.13314         270.00000         271.96661         -1.96661           54         Acenaphthylene         6.10516         270.00000         268.67840         10.22160	52	1,2,4,3-1ettamethylbezene	5.50129	218 00000	210 12022	-0.91100
53         Accuration         0.15514         2/0.0000         2/1.90001         -1.90001           54         Accuration         6.10516         270.00000         269.67940         10.22160	52	Aconomhthylono	6 12214	210.00000	219.12022	-1.12022
	55	Acenaphthene	6 10514	270.00000	2/1.90001	-1.90001

**Table 5.** Experimental and calculated with Eq. (4) values of hydrocarbon normal boiling points on training and test sets.

55	Fluoranthene	7.06943	383.00000	381.99941	1.00059
56	Pyrene	7.21102	393.00000	398.63907	-5.63907
57	Benzo(c)fluorene	7.24498	406.00000	402.63005	3.36995
58	Benzo(ghi)fluoranthene	7.57050	422.00000	440.88516	-18.88516
59	Benz(a)anthracene	7.55147	425.00000	438.64875	-13.64875
60	Dibenz(a,j)anthracene	8.32983	531.00000	530.12162	0.87838
61	Cyclopenta(cd)pyrene	7.54785	439.00000	438.22333	0.77667
62	Benzo(k)fluoranthene	7.89546	481.00000	479.07446	1.92554
63	Pervlene	8 02248	497 00000	494 00185	2 99815
64	Anthanthrene	8 46734	547 00000	546 28180	0 71820
65	Indeno(1.2.3-cd)pyrene	8 34709	534 00000	532 15002	1 84998
66	Dibenz(a c)anthracene	8 32983	535,00000	530 12162	4 87838
67	Picene	8 32983	519,00000	530 12162	-11 12162
68	Coronene	8 88997	590,00000	595 94927	-5 94927
69	Dibenzo(a i)pyrene	8 75909	594 00000	580 56826	13 43174
70	Dibenzo(a l)pyrene	8 75909	595,00000	580 56826	14 43174
10	Test set	0.70707	272.00000	200.20020	11.13171
1	4-Methylheptane	4 82193	117 70000	117 87321	-0 17321
2	n-Pentane	4 08366	36 10000	31 11172	4 98828
3	Dibenzo(a e)pyrene	8 75909	592,00000	580 56826	11 43174
4	Dibenzo(a,h)pyrene	8.75909	596.00000	580.56826	15.43174
5	Dibenz(a h)anthracene	8 32983	535,00000	530 12162	4 87838
6	Benzo(ghi)pervlene	8 46734	542,00000	546 28180	-4 28180
7	Indeno(1 2 3-cd)fluoranthene	8 34709	531,00000	532 15002	-1 15002
8	Benz(a)pyrene	8 02248	496 00000	494 00185	1 99815
9	Benzo(e)pyrene	8 02248	493 00000	494 00185	-1.00185
10	Naphthacene	7 55147	440 00000	438 64875	1 35125
11	Triphenylene	7 55147	429 00000	438 64875	-9 64875
12	Benzo(b)fluoranthene	7 89546	481 00000	479 07446	1 92554
13	Chrysene	7 55147	431 00000	438 64875	-7 64875
14	Benzo(a)fluorene	7.24498	403.00000	402.63005	0.36995
15	Benzo(b)fluorene	7.24498	398.00000	402.63005	-4.63005
16	Fluorene	6.33469	294.00000	295.65277	-1.65277
17	4H-Cyclopenta(def)phenanthrene	6.88941	359.00000	360.84346	-1.84346
18	Benzo(j)fluoranthene	7.89546	480.00000	479.07446	0.92554
19	Phenanthrene	6.68305	338.00000	336.59204	1.40796
20	Anthracene	6.68305	340.00000	336.59204	3.40796
21	1.4-Dimethyl-2-ethylbenzene	5.43194	186.90000	189.56159	-2.66159
22	1,2,3,5-Tetramethylbenzene	5.50129	198.20000	197.71160	0.48840
23	1,2-Dimethyl-4-ethylbenzene	5.43194	189.80000	189.56159	0.23841
24	1,3-Dimethyl-2-ethylbenzene	5.43194	190.00000	189.56159	0.43841
25	1-Methyl-2-n-propylbenzene	5.40986	184.80000	186.96675	-2.16675
26	1-Methyl-3-n-propylbenzene	5.40986	181.80000	186.96675	-5.16675
27	n-Butylbenzene	5.38770	183.30000	184.36250	-1.06250
28	1,2-Diethylbenzene	5.36168	183.40000	181.30463	2.09537
29	1,2,3-Trimethylbenzene	5.26149	176.10000	169.53030	6.56970
30	1,2,4-Trimethylbenzene	5.26149	169.40000	169.53030	-0.13030
31	n-Propylbenzene	5.16582	159.20000	158.28717	0.91283
32	1-Methyl-2-ethylbenzene	5.18892	165.20000	161.00188	4.19812
33	Ethylbenzene	4.93396	136.20000	131.03898	5.16102
34	o-Xylene	5.01022	144.40000	140.00105	4.39895
35	3,3,4-Trimethylhexane	4.97097	140.50000	135.38839	5.11161
36	2,3,4-Trimethylhexane	4.96909	139.00000	135.16746	3.83254
37	3,3-Dimethylheptane	5.01606	137.30000	140.68737	-3.38737
38	3,4-Dimethylheptane	5.01421	140.60000	140.46996	0.13004
39	2,3-Dimethylheptane	5.01421	140.50000	140.46996	0.03004
40	2,4-Dimethylheptane	5.01421	133.50000	140.46996	-6.96996
41	4-Methyloctane	5.05892	142.50000	145.72428	-3.22428
42	3-Ethylheptane	5.05892	143.00000	145.72428	-2.72428

43	3,4-Dimethylhexane	4.77500	117.70000	112.35800	5.34200
44	n-Nonane	5.10324	150.80000	150.93276	-0.13276
45	2,3,5-Trimethylhexane	4.96909	131.30000	135.16746	-3.86746
46	3-ethyl-2-methyl-hexane	5.01421	138.00000	140.46996	-2.46996
47	2,2,5-Trimethylhexane	4.97097	124.10000	135.38839	-11.28839
48	4,4-Dimethylheptane	5.01606	135.20000	140.68737	-5.48737
49	2,3-dimethyl-3-ethylpentane	4.97097	142.00000	135.38839	6.61161
50	2,2,3-Trimethylhexane	4.97097	133.60000	135.38839	-1.78839
51	2,2-dimethyl-3-ethylpentane	4.97097	133.80000	135.38839	-1.58839
52	2,3,3,4-Tetramethylpentane	4.92545	141.60000	130.03888	11.56112
53	3-Ethylhexane	4.82193	118.50000	117.87321	0.62679
54	n-Octane	4.86841	125.70000	123.33554	2.36446
55	2,5-Dimethylhexane	4.77500	109.10000	112.35800	-3.25800
56	2-Methylheptane	4.82193	117.60000	117.87321	-0.27321
57	2,3,4-Trimethylpentane	4.72760	113.50000	106.78755	6.71245
58	2,3-Dimethylhexane	4.77500	115.60000	112.35800	3.24200
59	2,2,4-Trimethylpentane	4.72957	99.20000	107.01907	-7.81907
60	2,2-Dimethylhexane	4.77694	106.80000	112.58599	-5.78599
61	n-Heptane	4.62165	98.40000	94.33631	4.06369
62	2,2,3,3-tetramethylbutane	4.68370	106.50000	101.62842	4.87158
63	2,4-Dimethylpentane	4.52315	80.50000	82.76059	-2.26059
64	2-Methylhexane	4.57267	90.00000	88.58018	1.41982
65	2,2,3-Trimethylbutane	4.47516	80.90000	77.12080	3.77920
66	2,2-Dimethylpentane	4.52521	79.20000	83.00268	-3.80268
67	2,3-Dimethylbutane	4.25643	58.00000	51.41565	6.58435
68	2-methylpentane	4.30901	60.30000	57.59486	2.70514
69	2,4-Dimethylhexane	4.77500	109.40000	112.35800	-2.95800
70	3-Methylheptane	4.82193	118.90000	117.87321	1.02679



Figure 1. Plot of experimental vs. calculated with Eq. (4) normal boiling points on the training set.



Figure 2. Plot of experimental vs. calculated with Eq. (4) normal boiling points on the test set.