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Research Article

Prediction of Normal Boiling Points of Hydrocarbons Using Simple Molecular Properties

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Abstract Four hundred and seventy-six hydrocarbons (C_nH_m) were utilized to fit their normal boiling point temperatures (NBPT) as a function of molecular weight and carbon atomic fraction. The proposed model is of the following form: NBPT $= a^*(C_{frac})\hat{}b^*(MW)\hat{}c$, where a, b, and c are the non-linear regressed parameters for the given model; C_{frac} is the carbon atomic fraction in a molecule, which is equal to $n/(n+m)$ for a hydrocarbon compound; and MW is the molecular weight, which is calculated as $12^*n + 1^*m$. The model was found to predict NBPT with an adequate accuracy, manifested via the associated percent relative error (PRE) of the curve-fitted NBPT. Out of the examined 476 hydrocarbons, methane, ethylene, and acetylene were found to have PRE values higher than 10%. If the confidence interval is further reduced to PRE value less than 5%, then 43 compounds will be excluded, and then NBPT for the other 433 compounds could be well predicted by the proposed model. Although the proposed model does not differentiate among isomers having the same molecular weight and chemical formula, nevertheless, the difference in NBPT among isomers is not really significant to be picked up by a simple, straightforward model. A more rigorous model will work hard to offset such small differences in NBPT among isomers, nevertheless, at the expense of model simplicity.

Keywords model; normal boiling point; hydrocarbons; carbon atoms; molecular formula; hydrocarbons

1 Introduction

The prediction of physicochemical properties like the normal boiling point temperature (NBPT) of a substance is a major target of computational chemistry. NBPT is one of the major physicochemical properties used to identify a compound. This property is a fundamental characteristic of chemical compounds, and it is involved in many correlations used to estimate thermo-physical properties. In fact, commercial simulators, like ASPEN PLUS®, can be used to identify, or fill in the gaps of, a molecule with given chemical formula; nevertheless, software packages require some properties of the compound as a priori. NBPT and standard liquid density are the most important properties, for such properties, along with group contribution methods, facilitate the estimation of other missing properties.

NBPT of a compound is related, in general, to its molecular structure; but the nature of the relationship is not straightforward. Different models were used to correlate the boiling points of homologous hydrocarbons with the number of carbon atoms or molecular weight [5]. The group contribution method, used for predicting NBPT, relies on the assumption that the cohesion forces in the liquid predominantly have a short-range character, and the complex molecule is sub-divided into predefined structural groups, each of which adds a constant increment to the value of a property for a compound. In general, the group contribution methods give good predictions of boiling points for small and non-polar molecules [4].

Ivanciuc et al. [3] used quantitative structure—property relationship (QSPR) models for the estimation of boiling points of organic compounds containing halogens, oxygen, or sulfur without hydrogen bonding, accompanied by the comprehensive descriptors for structural and statistical analysis (CODESSA). Using the multi-linear regression (MLR), the boiling points of 185 compounds containing oxygen or sulfur could be accurately computed with a MLR equation containing six theoretical descriptors and having the following statistical indices: $R^2 = 0.992$ and standard deviation of 6.3 °C. For a set of 534 halogenated alkanes C1–C4, the best MLR equation with five descriptors has $R^2 = 0.990$ and standard deviation of 9.0 °C. In their opinion, the QSPR models developed with CODESSA allowed accurate computation of the boiling points of organic compounds using simple constitutional, topological, electrostatic, and quantum indices that could be computed with standard quantum chemistry.

Cholakov et al. [2] proposed a correlation between the molecular structure and the normal boiling point of hydrocarbons. Its main features are the relative simplicity, sound predictions, and applicability to diversified industrially important structures, whose boiling points and numbers of

carbon atoms span a wide range. They used two types of descriptors: molecular energy and carbon atom descriptors. For the first type, a structure is treated as a collection of atoms held together by elastic (harmonic) forces-bonds, which constitute the force field. For the second type, it comprises the highest level of sophistication, like the graph topological indices, derived from the adjacency and distance matrices of a chemical structure and the lowest level of sophistication of carbon atom descriptors, like the numbers of atoms engaged in specific groups (atom counts).

Wang et al. [6] extended the application of conductor-like screening model-based segment activity coefficient model for boiling point calculation (COSMO-SAC-BP) solvation model to predict NBPT for environmentally significant substances that are large and more complex molecules, including pollutants, herbicides, insecticides, and drugs. The average absolute deviation in the predicted boiling points of these complex molecules, which spans the range of 266–708 K, was 17.8 K or 3.7%. They concluded that their 3.7% was similar to the value of 3.2% that was obtained for 369 molecules in their earlier study, indicating that this method could be applied well outside the systems used to train the model.

Chan et al. [1] proposed an empirical method for estimating the boiling points of organic molecules based on density functional theory (DFT) calculations with polarized continuum model (PCM) solvent corrections. The boiling points were calculated as the sum of three contributions. The first term was directly calculated from the structural formula of the molecule and was related to its effective surface area. The second was a measure of the electronic interactions between molecules, based on the DFT-PCM solvation energy, and the third was employed only for planar aromatic molecules. The method was found applicable to a very diverse range of organic molecules, with normal boiling points in the range of $-50\,^{\circ}\mathrm{C}$ to $500\,^{\circ}\mathrm{C}$, and included 10 different elements (C, H, Br, Cl, F, N, O, P, S, and Si).

In this model, the NBPT of a hydrocarbon compound is expressed as a function of simple molecular indicators, namely, the carbon atomic fraction ($\mathrm{C_{frac}}$) and molecular weight (*MW*). Such molecular indicators are really simple to calculate. For example, given methane ($\mathrm{CH_4}$), then its $\mathrm{C_{frac}}$ will be $1/(1+4) = 0.20$. Moreover, its *MW* is simply equal to $1\times 12+4\times 1 = 16$. On the other hand, the difference in NBPT among isomers having the same $\mathrm{C_{frac}}$ and *MW* was found to be small. Any attempt to account for such small differences among isomers will be at the expense of model simplicity.

2 Model development

Four hundred and seventy-six hydrocarbon compounds were used in the non-linear regression process for finding the best fit for their normal boiling point properties. The database of hydrocarbon compounds includes the following categories:

(1) Normal paraffin: example: n-alkane.
(2) Non-normal paraffin: example: iso-alkane, methyl-alkane, ethyl-alkane, and methyl-ethyl-alkane.
(3) Naphthene: the major structure is saturated ring; example: cyclo-alkane.
(4) Olefin: contains a single C=C double bond; example: alkene, methyl-alkene, ethyl-alkene, and di-methyl-alkene.
(5) Diolefin: contains two C=C double bonds; example: alkadiene, methyl-alkadiene, and ethyl-alkadiene.
(6) Cyclic olefin: contains a single C=C double bond within the otherwise saturated ring; example: cyclo-alkene, methyl-cyclo-alkene, and ethyl-cyclo-alkene.
(7) Alkyne: contains a C≡C triple bond between carbons; example: acetylene, methyl acetylene, pentyne, and hexyne.
(8) Aromatic: contains a single ring; example: benzene, toluene, and xylene.
(9) Aromatic with attached olefin side chain: example: Styrene, ethenyl-benzene, and propenyl-benzene.
(10) Aromatic with multiple rings directly connected by C−C bonds between the rings: example: bi-phenyl and 1-methyl-2-phenylbenzene.
(11) Aromatic with multiple rings connected through other saturated carbon species: example: di-phenyl-methane and 1,1-di-phenyl-dodecane.
(12) Aromatic with multiple rings connected through other carbon species with triple bond: example: di-phenyl-acetylene.
(13) Aromatic with multiple condensed rings: example: naphthalene, pyrene, methyl-naphthalene, and nonyl-naphthalene.
(14) Aromatic with attached saturated rings: examples: 1,2,3,4-tetra-hydro-naphthalene and 1-methyl-2,3-dihydro-indene.
(15) Aromatic with attached unsaturated (but not aromatic) rings: example: indene and 1-methyl-indene.

The carbon atomic fraction (X) and molecular weight (Y) were chosen as the independent variables, and the NBPT represented the dependent variable (Z) from regression point of view:

$$Z = a\times(X)^b\times(Y)^c = \mathrm{NBPT} = a(\mathrm{C_{frac}})^b\times(MW)^c. \quad (1)$$

For example, given methane ($\mathrm{CH_4}$), then its $\mathrm{C_{frac}}$ will be $1/(1+4) = 0.20$. Moreover, its *MW* is simply equal to $1\times 12+4\times 1 = 16$.

The results of non-linear regression for (1), with 95% confidence interval, are:

$$Z = \mathrm{NBPT} = (49.5\mp 0.24)\times\left(\mathrm{C_{frac}}\right)^{(0.2791\pm 0.0021)} \times(MW)^{(0.5039\pm 0.0008)}. \quad (2)$$

Table 1: Small size molecules, like methane, ethylene, and acetylene were found to have PRE higher than 10%.

Database SN[a]	Compound	Formula	PRE (%)
1	Methane	CH_4	14.6%
191	Ethylene	C_2H_4	15.4%
321	Acetylene	C_2H_2	11.5%

[a]SN: Serial number in the API database of hydrocarbons.

The goodness of fit for (2) is given by *R-square* as 0.9997 and adjusted *R-square* as 0.9997 with the sum of squared error (SSE) of 1,796 K^2 and root mean squared error (RMSE) of 1.949 K. The RMSE is essentially the standard error in MATLAB® notation.

The PRE is defined as:

$$\text{PRE} = \frac{|\text{Curve-fitted NBPT} - \text{Experimental NBPT}|}{\text{Experimental NBPT}} \times 100\%. \quad (3)$$

From engineering applications standpoint, it is tolerated to have uncertainty associated with a measured or calculated quantity, which amounts to a maximum PRE value of 10%.

3 Results and discussion

The mean PRE for all examined compounds was found to be 2.07, with a standard error of 2.1. However, Table 1 shows three compounds that have PRE higher than 10%.

Other than that, the model could predict well the normal boiling point temperature of a hydrocarbon as a function of its molecular size and carbon atomic (mole) fraction.

Figure 1 shows the plot of the curve-fitted NBPT versus the experimental NBPT for all examined 476 hydrocarbons. Most of the data points fall on the 45° diagonal ($Y = X$). There is, however, a small deviation in the high-boiling point region. Figure 2 shows that only three data points lie above the 10% PRE datum. In fact, if we take our datum to be 5% not 10%, then we will exclude only 43 compounds with PRE higher than 5%. The 43 compounds that have PRE > 5.0 are shown in Table 2. The appendix contains all hydrocarbons used in this study.

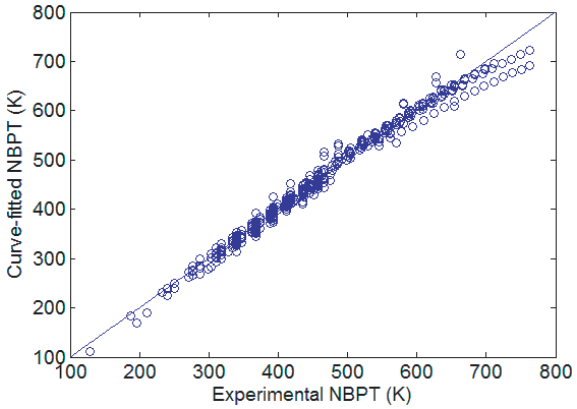

Figure 1: Plot of the curve-fitted NBPT versus the experimental NBPT for all examined 476 hydrocarbons.

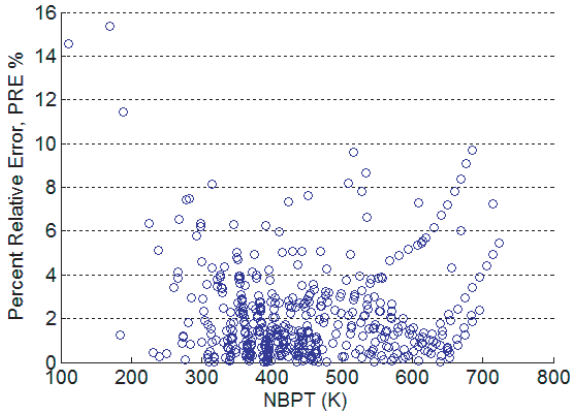

Figure 2: The PRE for all examined 476 hydrocarbons.

On the other hand, regarding the isomers or stereochemistry of molecules, an example is shown here to demonstrate the strength and weakness of the model. Table 3 shows 17 different isomers that have the same chemical formula, that is, C_8H_{18} and molecular weight of 114.23.

Table 2: Forty-three compounds with PRE higher than 5%.

#	SN	Compound	Formula	PRE (%)
1	1	Methane	CH_4	14.5595
2	30	*n*-triacontane	$C_{30}H_{62}$	5.4471
3	33	Neopentane	C_5H_{12}	7.4944
4	90	2,2,5,5-tetramethylhexane	$C_{10}H_{22}$	5.9635
5	178	Cycloheptane	C_7H_{14}	6.2384
6	179	Cyclooctane	C_8H_{16}	7.3618
7	180	Cyclononane	C_9H_{18}	7.6306
8	183	Cis-decahydronaphthalene	$C_{10}H_{18}$	5.0833
9	185	1-methyl-[cis-decahydro-naphthalene]	$C_{11}H_{20}$	9.6191
10	186	1-methyl-[trans-decahydro-naphthalene]	$C_{11}H_{20}$	8.1962
11	187	1-ethyl-[cis-decahydro-naphthalene]	$C_{12}H_{22}$	8.6644
12	188	1-ethyl-[trans-decahydro-naphthalene]	$C_{12}H_{22}$	7.7997

Table 2: To be continued.

#	SN	Compound	Formula	PRE (%)
13	191	Ethylene	C_2H_4	15.3562
14	192	Propylene	C_3H_6	6.3560
15	201	3-methyl-1-butene	C_5H_{10}	5.7819
16	218	3,3-dimethyl-1-butene	C_6H_{12}	8.1481
17	247	4,4-dimethyl-1-pentene	C_7H_{14}	6.3129
18	253	Trans-4,4-dimethyl-2-pentene	C_7H_{14}	5.0300
19	289	Propadiene	C_3H_4	5.1350
20	291	1,3-butadiene	C_4H_6	6.5436
21	295	1,4-pentadiene	C_5H_8	6.3488
22	318	Dicyclopentadiene	$C_{10}H_{12}$	5.0799
23	319	Alpha-pinene	$C_{10}H_{16}$	5.0768
24	321	Acetylene	C_2H_2	11.4610
25	325	Vinylacetylene	C_4H_4	7.4442
26	328	3-methyl-1-butyne	C_5H_8	6.2127
27	408	1,1-diphenylhexane	$C_{18}H_{22}$	5.1471
28	409	1,1-dipmenylheptane	$C_{19}H_{24}$	5.3710
29	410	1,1-diphenyloctane	$C_{20}H_{26}$	5.7067
30	411	1,1-diphenylnonane	$C_{21}H_{28}$	6.1533
31	412	1,1-diphenyldecane	$C_{22}H_{30}$	6.7123
32	413	1,1-dipmenylundecane	$C_{23}H_{32}$	7.2137
33	414	1,1-diphenyldodecane	$C_{24}H_{34}$	7.8285
34	415	1,1-diphenyltridecane	$C_{25}H_{36}$	8.3921
35	416	1,1-diphenyltetradecane	$C_{26}H_{38}$	9.0689
36	417	1,1-diphenylpentadecane	$C_{27}H_{40}$	9.6972
37	418	Cis-1,2-diphenylethene	$C_{14}H_{12}$	6.6479
38	420	Phenylacetylene	C_8H_6	5.0306
39	422	1,2-diphenylbenzene	$C_{18}H_{14}$	7.3042
40	472	Anthracene	$C_{14}H_{10}$	5.5665
41	473	Phenanthrene	$C_{14}H_{10}$	5.4280
42	474	Pyrene	$C_{16}H_{10}$	6.0386
43	476	Chrysene	$C_{18}H_{12}$	7.2446

Table 3: Seventeen different stereo-chemical compounds with the same molecular weight (114.3) and chemical formula (C_8H_{18}). The minimum, maximum, and mean of NBPT (K) is shown at the bottom.

#	Compound	Experimental NBPT (K)		
1	2-methylheptane	390.79		
2	3-methylheptane	392.07		
3	4-methylheptane	390.86		
4	3-ethylhexane	391.68		
5	2,2-dimethylhexane	379.99		
6	2,3-dimethylhexane	388.76		
7	2,4-dimethylhexane	382.58		
8	2,5-dimethylhexane	382.26		
9	3,3-dimethylhexane	385.12		
10	3,4-dimethylhexane	390.88		
11	2-methyl-3-ethylpentane	388.80		
12	3-methyl-3-ethylpentane	391.41		
13	2,2,3-trimethylpentane	382.99		
14	2,2,4-trimethylpentane	372.39		
15	2,3,3-trimethylpentane	387.92		
16	2,3,4-trimethylpentane	386.62		
17	2,2,3,3-tetramethylbutane	379.62		
			Predicted	PRE (%)
	Minimum	372.39	387.8	4.1
	Maximum	392.07	387.8	1.1
	Mean	386.16	387.8	0.4

Based on the proposed model (2), the predicted NBPT is:

$$\begin{aligned}\text{NBPT} &= (49.5) \times (0.30769)^{(0.2791)} \times (114.23)^{(0.5039)} \\ &= 387.8\,\text{K}.\end{aligned}$$

This means that the value given by the proposed model matches well the mean value shown in Table 3, with a PRE value of 0.4%. As Table 3 shows, the maximum PRE (%) is found to be 4.1% for such a set of stereo-chemical compounds. Moreover, in the previous set, the maximum percent relative difference occurs between the lowest and mean of experimental NBPT:

$$\frac{(386.2 - 372.4)}{386.2} \times 100\% = 3.6\%.$$

So strictly speaking, it is true that the proposed model does not differentiate among isomers of the same molecular weight and chemical formula; however, at the same time, a maximum percent relative difference of 3.6% is really hardly noticeable by this model. A more rigorous model will work hard to offset this 3.6% value, but at the expense of model simplicity.

4 Conclusion

The NBPT for a hydrocarbon compound could be expressed as a function of simple molecular properties with an adequate accuracy manifested via the associated PRE of the curve-fitted NBPT. It is very easy for the user to calculate both the molecular weight and the carbon atomic fraction for a given chemical formula of a hydrocarbon (C_nH_m). Out of the examined 476 hydrocarbons, methane, ethylene, and acetylene were found to have PRE values higher than 10%. If the confidence interval is further confined down to PRE value less than 5%, then 43 compounds will be excluded, and then NBPT for the other 433 compounds could be well predicted by the proposed model. Consequently, in fulfillment of the acceptable engineering accuracy, one can say that the model adequately predicts NBPT for each of 433 different hydrocarbons with PRE less than 5% for each.

Appendix

List of 476 hydrocarbons used in the non-linear regression process to express the normal boiling point temperature as a function of hydrocarbon molecular weight and its carbon atomic fraction.

DB SN	Compound	Formula	DB SN	Compound	Formula
1	Methane	CH_4	29	n-nonacosane	$C_{29}H_{60}$
2	Ethane	C_2H_6	30	n-triacontane	$C_{30}H_{62}$
3	Propane	C_3H_8	31	Isobutane	C_4H_{10}
4	n-butane	C_4H_{10}	32	Isopentane	C_5H_{12}
5	n-pentane	C_5H_{12}	33	Neopentane	C_5H_{12}
6	n-hexane	C_6H_{14}	34	2-methylpentane	C_6H_{14}
7	n-heptane	C_7H_{16}	35	3-methylpentane	C_6H_{14}
8	n-octane	C_8H_{18}	36	2,2-dimethylbutane	C_6H_{14}
9	n-nonane	C_9H_{20}	37	2,3-dimethylbutane	C_6H_{14}
10	n-decane	$C_{10}H_{22}$	38	2-methylhexane	C_7H_{16}
11	n-undecane	$C_{11}H_{24}$	39	3-methylhexane	C_7H_{16}
12	n-dodecane	$C_{12}H_{26}$	40	3-ethylpentane	C_7H_{16}
13	n-tridecane	$C_{13}H_{28}$	41	2,2-dimethylpentane	C_7H_{16}
14	n-tetradecane	$C_{14}H_{30}$	42	2,3-dimethylpentane	C_7H_{16}
15	n-pentadecane	$C_{15}H_{32}$	43	2,4-dimethylpentane	C_7H_{16}
16	n-hexadecane	$C_{16}H_{34}$	44	3,3-dimetmylpentane	C_7H_{16}
17	n-heptadecane	$C_{17}H_{36}$	45	2,2,3-trimethylbutane	C_7H_{16}
18	n-octadecane	$C_{18}H_{38}$	46	2-methylheptane	C_8H_{18}
19	n-nonadecane	$C_{19}H_{40}$	47	3-methylheptane	C_8H_{18}
20	n-eicosane	$C_{20}H_{42}$	48	4-methylheptane	C_8H_{18}
21	n-heneicosane	$C_{21}H_{44}$	49	3-ethylhexane	C_8H_{18}
22	n-docosane	$C_{22}H_{46}$	50	2,2-dimethylhexane	C_8H_{18}
23	n-tricosane	$C_{23}H_{48}$	51	2,3-dimethylhexane	C_8H_{18}
24	n-tetracosane	$C_{24}H_{50}$	52	2,4-dimethylhexane	C_8H_{18}
25	n-pentacosane	$C_{25}H_{52}$	53	2,5-dimethylhexane	C_8H_{18}
26	n-hexacosane	$C_{26}H_{54}$	54	3,3-dimethylhexane	C_8H_{18}
27	n-heptacosane	$C_{27}H_{56}$	55	3,4-dimethylhexane	C_8H_{18}
28	n-octacosane	$C_{28}H_{58}$	56	2-methyl-3-ethylpentane	C_8H_{18}

DB SN	Compound	Formula	DB SN	Compound	Formula
57	3-methyl-3-ethylpentane	C_8H_{18}	112	Trans-l-methyl-2-ethyl-cyclopentane	C_8H_{16}
58	2,2,3-trimethylpentane	C_8H_{18}	113	Cis-l-methyl-3-ethyl-cyclopentane	C_8H_{16}
59	2,2,4-trimethylpentane	C_8H_{18}	114	Trans-1-methyl-3-ethyl-cyclopentane	C_8H_{16}
60	2,3,3-trimethylpentane	C_8H_{18}	115	1,1,2-trimetmylcyclopentane	C_8H_{16}
61	2,3,4-trimethylpentane	C_8H_{18}	116	1,1,3-trimetmylcyclopentane	C_8H_{16}
62	2,2,3,3-tetramethylbutane	C_8H_{18}	117	l,cis-2,cis-3-trimethyl-cyclopentane	C_8H_{16}
63	2-methyloctane	C_9H_{20}	118	l,cis-2,trans-3-trimethyl-cyclopentane	C_8H_{16}
64	3-methyloctane	C_9H_{20}	119	l,trans-2,cis-3-trimethyl-cyclopentane	C_8H_{16}
65	4-methyloctane	C_9H_{20}	120	l,cis-2,cis-4-trimethyl-cyclopentane	C_8H_{16}
66	3-ethylheptane	C_9H_{20}	121	l,cis-2,trans-4-trimetmyl-cyclopentane	C_8H_{16}
67	2,2-dimethylheptane	C_9H_{20}	122	l,trans-2,cis-4-trimethyl-cyclopentane	C_8H_{16}
68	2,6-dimethylheptane	C_9H_{20}	123	n-butylcyclopentane	C_9H_{18}
69	2,2,3-trimethylhexane	C_9H_{20}	124	Isobutylcyclopentane	C_9H_{18}
70	2,2,4-trimethylhexane	C_9H_{20}	125	1-methyl-1-n-propyl-cyclopentane	C_9H_{18}
71	2,2,5-trimethylhexane	C_9H_{20}	126	1,1-diethylcyclopentane	C_9H_{18}
72	2,3,3-trimethylhexane	C_9H_{20}	127	Cis-1,2-diethylcyclopentane	C_9H_{18}
73	2,4,4-trimethylhexane	C_9H_{20}	128	1,1-dimethyl-2-ethyl-cyclopentane	C_9H_{18}
74	3,3,4-trimethylhexane	C_9H_{20}	129	n-pentylcyclopentane	$C_{10}H_{20}$
75	3,3-diethylpentane	C_9H_{20}	130	n-hexylcyclopentane	$C_{11}H_{22}$
76	2,2-dimethyl-3-ethylpentane	C_9H_{20}	131	n-heptylcyclopentane	$C_{12}H_{24}$
77	2,4-dimethyl-3-ethylpentane	C_9H_{20}	132	n-octylcyclopentane	$C_{13}H_{26}$
78	2,2,3,3-tetramethylpentane	C_9H_{20}	133	n-nonylcyclopentane	$C_{14}H_{28}$
79	2,2,3,4-tetramethylpentane	C_9H_{20}	134	n-decylcyclopentane	$C_{15}H_{30}$
80	2,2,4,4-tetramethylpentane	C_9H_{20}	135	n-undecylcyclopentane	$C_{16}H_{32}$
81	2,3,3,4-tetramethylpentane	C_9H_{20}	136	n-oodecylcyclopentane	$C_{17}H_{34}$
82	2-methylnonane	$C_{10}H_{22}$	137	n-trrdecylcyclopentane	$C_{18}H_{36}$
83	3-methylnonane	$C_{10}H_{22}$	138	n-tetradecylcyclopentane	$C_{19}H_{38}$
84	4-methylnonane	$C_{10}H_{22}$	139	n-pentadecylcyclopentane	$C_{20}H_{40}$
85	5-methylnonane	$C_{10}H_{22}$	140	n-hexadecylcyclopentane	$C_{21}H_{42}$
86	2,7-dimethyloctane	$C_{10}H_{22}$	141	n-heptadecylcyclopentane	$C_{22}H_{44}$
87	3,3,4-trimethylheptane	$C_{10}H_{22}$	142	n-octadecylcyclopentane	$C_{23}H_{46}$
88	3,3,5-trimethylheptane	$C_{10}H_{22}$	143	n-nonadecylcyclopentane	$C_{24}H_{48}$
89	2,2,3,3-tetramethylhexane	$C_{10}H_{22}$	144	n-eicosylcyclopentane	$C_{25}H_{50}$
90	2,2,5,5-tetramethylhexane	$C_{10}H_{22}$	145	Cyclohexane	C_6H_{12}
91	2,4-dimethyl-3-isopropyl-pentane	$C_{10}H_{22}$	146	Methylcyclohexane	C_7H_{14}
92	Cyclopropane	C_3H_6	147	Ethylcyclohexane	C_8H_{16}
93	Methylcyclopropane	C_4H_8	148	1,1-dimethylcyclohexane	C_8H_{16}
94	Ethylcyclopropane	C_5H_{10}	149	Cis-1,2-dimethylcyclohexane	C_8H_{16}
95	Cis-1,2-dimethylcyclopropane	C_5H_{10}	150	TRANS-1,2-dimethylcyclohexane	C_8H_{16}
96	Trans-1,2-dimethylcyclopropane	C_5H_{10}	151	CIS-I,3-dimetmylcyclohexane	C_8H_{16}
97	Cyclobutane	C_4H_8	152	Trans-1,3-dimethylcyclohexane	C_8H_{16}
98	Methylcyclobutane	C_5H_{10}	153	Cis-I,4-dimethylcyclohexane	C_8H_{16}
99	Ethylcyclobutane	C_6H_{12}	154	Trans-1,4-dimethylcyclohexane	C_8H_{16}
100	Cyclopentane	C_5H_{10}	155	n-propylcyclohexane	C_9H_{18}
101	Methylcyclopentane	C_6H_{12}	156	Isopropylcyclohexane	C_9H_{18}
102	Ethylcyclopentane	C_7H_{14}	157	n-butylcyclohexane	$C_{10}H_{20}$
103	1,1-dimethylcyclopentane	C_7H_{14}	158	isobutylcyclohexane	$C_{10}H_{20}$
104	Cis-1,2-dimethylcyclopentane	C_7H_{14}	159	Sec-butylcyclohexane	$C_{10}H_{20}$
105	Trans-1,2-dimethylcyclopentane	C_7H_{14}	160	Tert-butylcyclohexane	$C_{10}H_{20}$
106	Cis-1,3-dimethylcyclopentane	C_7H_{14}	161	1-methyl-4-isopropyl-cyclohexane	$C_{10}H_{20}$
107	Trans-1,3-dimethylcyclopentane	C_7H_{14}	162	n-pentylcyclohexane	$C_{11}H_{22}$
108	n-propylcyclopentane	C_8H_{16}	163	n-hexylcyclohexane	$C_{12}H_{24}$
109	Isopropylcyclopentane	C_8H_{16}	164	n-heptylcyclohexane	$C_{13}H_{26}$
110	1-methyl-1-ethylcyclopentane	C_8H_{16}	165	n-octylcyclohexane	$C_{14}H_{28}$
111	Cis-l-methyl-2-ethyl-cyclopentane	C_8H_{16}	166	n-nonylcyclohexane	$C_{15}H_{30}$

DB SN	Compound	Formula	DB SN	Compound	Formula
167	n-decylcyclohexame	$C_{16}H_{32}$	222	Trans-2-heptene	C_7H_{14}
168	n-undecylcyclohexane	$C_{17}H_{34}$	223	Cis-3-heptene	C_7H_{14}
169	n-dodecylcyclohexane	$C_{18}H_{36}$	224	Trans-3-heptene	C_7H_{14}
170	n-tridecylcyclohexane	$C_{19}H_{38}$	225	2-methyl-1-hexene	C_7H_{14}
171	n-tetradecylcyclohexane	$C_{20}H_{40}$	226	3-methyl-1-hexene	C_7H_{14}
172	n-pentadecylcyclohexane	$C_{21}H_{42}$	227	4-methyl-1-hexene	C_7H_{14}
173	n-hexadecylcyclohexane	$C_{22}H_{44}$	228	5-methyl-1-hexene	C_7H_{14}
174	n-meptadecylcyclohexane	$C_{23}H_{46}$	229	2-methyl-2-hexene	C_7H_{14}
175	n-octadecylcyclohexane	$C_{24}H_{48}$	230	Cis-3-methyl-2-hexene	C_7H_{14}
176	n-nonadecylcyclohexane	$C_{25}H_{50}$	231	Trans-3-methyl-2-hexene	C_7H_{14}
177	n-eicosylcyclohexane	$C_{26}H_{52}$	232	CIS-4-methyl-2-hexene	C_7H_{14}
178	Cycloheptane	C_7H_{14}	233	Trans-4-methyl-2-hexene	C_7H_{14}
179	Cyclooctane	C_8H_{16}	234	Cis-5-methyl-2-hexene	C_7H_{14}
180	Cyclononane	C_9H_{18}	235	Trans-5-methyl-2-hexene	C_7H_{14}
181	Ethylcycloheptane	C_9H_{18}	236	Trans-2-methyl-3-hexene	C_7H_{14}
182	Bicyclohexyl	$C_{12}H_{22}$	237	Trans-2-methyl-3-hexene	C_7H_{14}
183	CIS-decahydronaphthalene	$C_{10}H_{18}$	238	Cis-3-methyl-3-hexene	C_7H_{14}
184	Trans-decahydronaphtmalene	$C_{10}H_{18}$	239	Trans-3-methyl-3-hexene	C_7H_{14}
185	1-methyl-[cis-decahydro-naphthalene]	$C_{11}H_{20}$	240	2-ethyl-1-pentene	C_7H_{14}
186	1-methyl-[trans-decahydro-naphthalene]	$C_{11}H_{20}$	241	3-ethyl-1-pentene	C_7H_{14}
187	1-ethyl-[cis-decahydro-naphthalene]	$C_{12}H_{22}$	242	3-ethyl-2-pentene	C_7H_{14}
188	1-ethyl-[trans-decahydro-naphthalene]	$C_{12}H_{22}$	243	2,3-dimethyl-1-pentene	C_7H_{14}
189	9-ethyl-[cis-decahydronaphthalene]	$C_{12}H_{22}$	244	2,4-dimethyl-1-pentene	C_7H_{14}
190	9-ethyl-[trans-decahydro-naphthalene]	$C_{12}H_{22}$	245	3,3-dimethyl-1-pentene	C_7H_{14}
191	Ethylene	C_2H_4	246	3,4-dimethyl-1-pentene	C_7H_{14}
192	Propylene	C_3H_6	247	4,4-dimethyl-1-pentene	C_7H_{14}
193	1-butene	C_4H_8	248	2,3-dimethyl-2-pentene	C_7H_{14}
194	Cis-2-butene	C_4H_8	249	2,4-dimethyl-2-pentene	C_7H_{14}
195	Trans-2-butene	C_4H_8	250	Cis-3,4-dimethyl-2-pentene	C_7H_{14}
196	Isobutene	C_4H_8	251	Trans-3,4-dimethyl-2-pentene	C_7H_{14}
197	1-pentene	C_5H_{10}	252	Cis-4,4-dimethyl-2-pentene	C_7H_{14}
198	Cis-2-pentene	C_5H_{10}	253	Trans-4,4-dimethyl-2-pentene	C_7H_{14}
199	Trans-2-pentene	C_5H_{10}	254	3-methyl-2-ethyl-1-buteme	C_7H_{14}
200	2-methyl-1-butene	C_5H_{10}	255	2,3,3-trimethyl-1-butene	C_7H_{14}
201	3-methyl-1-butene	C_5H_{10}	256	1-octene	C_8H_{16}
202	2-methyl-2-butene	C_5H_{10}	257	Trans-2-octene	C_8H_{16}
203	1-hexene	C_6H_{12}	258	Trans-2-octene	C_8H_{16}
204	Cis-2-hexene	C_6H_{12}	259	Trans-3-octene	C_8H_{16}
205	Trans-2-hexene	C_6H_{12}	260	Trans-3-octene	C_8H_{16}
206	Cis-3-hexene	C_6H_{12}	261	Trans-4-octene	C_8H_{16}
207	Trans-3-hexene	C_6H_{12}	262	Trans-4-octene	C_8H_{16}
208	2-methyl-1-pentene	C_6H_{12}	263	2-methyl-1-heptene	C_8H_{16}
209	3-methyl-1-pentene	C_6H_{12}	264	3-methyl-1-heptene	C_8H_{16}
210	4-methyl-1-pentene	C_6H_{12}	265	4-methyl-1-heptene	C_8H_{16}
211	2-methyl-2-pentene	C_6H_{12}	266	Trans-6-metmyl-2-heptene	C_8H_{16}
212	Cis-3-methyl-2-pentene	C_6H_{12}	267	Trans-3-methyl-3-heptene	C_8H_{16}
213	Trans-3-methyl-2-pentene	C_6H_{12}	268	2-ethyl-1-hexene	C_8H_{16}
214	Cis-4-methyl-2-pentene	C_6H_{12}	269	3-ethyl-1-hexene	C_8H_{16}
215	Trans-4-methyl-2-pentene	C_6H_{12}	270	4-ethyl-1-hexene	C_8H_{16}
216	2-ethyl-1-butene	C_6H_{12}	271	2,3-dimethyl-1-hexene	C_8H_{16}
217	2,3-dimethyl-1-butene	C_6H_{12}	272	2,3-dimethyl-2-hexene	C_8H_{16}
218	3,3-dimethyl-1-butene	C_6H_{12}	273	Cis-2,2-dimethyl-3-hexene	C_8H_{16}
219	2,3-dimethyl-2-butene	C_6H_{12}	274	2,3,3-trimethyl-1-pentene	C_8H_{16}
220	1-heptene	C_7H_{14}	275	2,4,4-trimethyl-1-pentene	C_8H_{16}
221	Cis-2-heptene	C_7H_{14}	276	2,4,4-trimethyl-2-pentene	C_8H_{16}

DB SN	Compound	Formula	DB SN	Compound	Formula
277	1-nonene	C_9H_{18}	332	1-nomyne	C_9H_{16}
278	1-decene	$C_{10}H_{20}$	333	1-decyne	$C_{10}H_{18}$
279	1-undecene	$C_{11}H_{22}$	334	Benzene	C_6H_6
280	1-dodecene	$C_{12}H_{24}$	335	Toluene	C_7H_8
281	1-tridecene	$C_{13}H_{26}$	336	Ethylbenzene	C_8H_{10}
282	1-tetradecene	$C_{14}H_{28}$	337	O-xylene	C_8H_{10}
283	1-pentadecene	$C_{15}H_{30}$	338	M-xylene	C_8H_{10}
284	1-hexadecene	$C_{16}H_{32}$	339	P-xylene	C_8H_{10}
285	1-heptadecene	$C_{17}H_{34}$	340	n-propylbenzene	C_9H_{12}
286	1-octadecene	$C_{18}H_{36}$	341	Isopropylbenzene	C_9H_{12}
287	1-nonadecene	$C_{19}H_{38}$	342	O-ethyltoluene	C_9H_{12}
288	1-eicosene	$C_{20}H_{40}$	343	M-ethyltoluene	C_9H_{12}
289	Propadiene	C_4H_6	344	P-ethyltoluene	C_9H_{12}
290	1,2-butadiene	C_4H_6	345	1,2,3-trimethylbenzene	C_9H_{12}
291	1,3-butadiene	C_4H_6	346	1,2,4-trimethylbenzene	C_9H_{12}
292	1,2-pentadiene	C_5H_8	347	1,3,5-trimethylbenzene	C_9H_{12}
293	Cis-1,3-pentaorene	C_5H_8	348	n-butylbenzene	$C_{10}H_{14}$
294	Trans-1,3-pentadiene	C_5H_8	349	Isobutylbenzene	$C_{10}H_{14}$
295	1,4-pentadiene	C_5H_8	350	Sec-butylbenzene	$C_{10}H_{14}$
296	2,3-pentadiene	C_5H_8	351	Tert-butylbenzene	$C_{10}H_{14}$
297	3-methyl-1,2-butadiene	C_5H_8	352	1-methyl-2-n-propylbenzene	$C_{10}H_{14}$
298	2-methyl-1,3-butadiene	C_5H_8	353	1-methyl-3-n-propylbenzene	$C_{10}H_{14}$
299	2,3-dimethyl-1,3-butadiene	C_6H_{10}	354	1-metmyl-4-n-propylbenzene	$C_{10}H_{14}$
300	1,2-hexadiene	C_6H_{10}	355	O-cymene	$C_{10}H_{14}$
301	1,5-hexadiene	C_6H_{10}	356	M-cymene	$C_{10}H_{14}$
302	2,3-hexadiene	C_6H_{10}	357	P-cynene	$C_{10}H_{14}$
303	3-methyl-1,2-pentadiene	C_6H_{10}	358	O-diethylbenzene	$C_{10}H_{14}$
304	2-methyl-1,5-hexadiene	C_7H_{12}	359	M-diethylbenzene	$C_{10}H_{14}$
305	2-methyl-2,4-hexadiene	C_7H_{12}	360	P-diethylbenzene	$C_{10}H_{14}$
306	2,6-octadiene	C_8H_{14}	361	1,2-dimethyl-3-ethylbenzene	$C_{10}H_{14}$
307	2,6-dimethyl-1,5-heptadiene	C_9H_{16}	362	1,2-dimethyl-4-ethylbenzene	$C_{10}H_{14}$
308	3,7-dimethyl-1,6-octaoiene	$C_{10}H_{18}$	363	1,3-dimethyl-2-ethylbenzene	$C_{10}H_{14}$
309	Cyclopentene	C_5H_8	364	1,3-dimethyl-4-ethylbenzene	$C_{10}H_{14}$
310	1-methyl-cyclopentene	C_6H_{10}	365	1,3-dimethyl-5-ethylbenzene	$C_{10}H_{14}$
311	1-ethylcyclopentene	C_7H_{12}	366	1,4-dimethyl-2-ethylbenzene	$C_{10}H_{14}$
312	3-ethylcyclopentene	C_7H_{12}	367	1,2,3,4-tetramethylbenzene	$C_{10}H_{14}$
313	1-n-propylcyclopentene	C_8H_{14}	368	1,2,3,5-tetramethylbenzene	$C_{10}H_{14}$
314	Cyclohexene	C_6H_{10}	369	1,2,4,5-tetramethylbenzene	$C_{10}H_{14}$
315	1-methylcyclohexene	C_7H_{12}	370	n-pentylbenzene	$C_{11}H_{16}$
316	1-ethylcyclohexene	C_8H_{14}	371	n-hexylbenzene	$C_{12}H_{18}$
317	Cyclopentadiene	C_5H_6	372	n-heptylbenzene	$C_{13}H_{20}$
318	Dicyclopentadiene	$C_{10}H_{12}$	373	n-octylbenzene	$C_{14}H_{22}$
319	Alpha-pinene	$C_{10}H_{16}$	374	n-nonylbenzene	$C_{15}H_{24}$
320	Beta-pinene	$C_{10}H_{16}$	375	n-decylbenzene	$C_{16}H_{26}$
321	Acetylene	C_2H_2	376	n-undecylbenzene	$C_{17}H_{28}$
322	Methylacetylene	C_4H_6	377	n-dodecylbenzene	$C_{18}H_{30}$
323	Dimethylacetylene	C_4H_6	378	n-tridecylbenzene	$C_{19}H_{32}$
324	Ethylacetylene	C_4H_6	379	n-tetradecylbenzene	$C_{20}H_{34}$
325	Vinylacetylene	C_4H_4	380	n-pentadecylbenzene	$C_{21}H_{36}$
326	1-pentyne	C_5H_8	381	n-hexadecylbenzene	$C_{22}H_{38}$
327	2-pentyne	C_5H_8	382	Cyclohexylbenzene	$C_{12}H_{16}$
328	3-methyl-1-butyne	C_5H_8	383	Styrene	C_8H_8
329	1-hexyne	C_6H_{10}	384	Cis-l-propenyl benzene	C_9H_{10}
330	1-heptyne	C_7H_{12}	385	Trans-l-propenyl benzene	C_9H_{10}
331	1-octyne	C_8H_{14}	386	2-propenyl benzene	C_9H_{10}

DB SN	Compound	Formula	DB SN	Compound	Formula
387	1-methyl-2-ethenyl benzene	C_9H_{10}	432	1-n-propylnaphthalene	$C_{13}H_{14}$
388	1-methyl-3-ethenyl benzene	C_9H_{10}	433	2-n-propylnaphthalene	$C_{13}H_{14}$
389	1-methyl-4-ethenyl benzene	C_9H_{10}	434	1-n-butylnaphthalene	$C_{14}H_{16}$
390	1-methyl-4-(trans-1-n-propenyl)benzene	$C_{10}H_{12}$	435	2-N-butylnaphthalene	$C_{14}H_{16}$
391	1-ethyl-2-ethenyl benzene	$C_{10}H_{12}$	436	1-n-pentylnaphthalene	$C_{15}H_{18}$
392	l-ethyl-3-ethenyl benzene	$C_{10}H_{12}$	437	1-n-hexylnaphthalene	$C_{16}H_{20}$
393	l-ethyl-4-ethenyl benzene	$C_{10}H_{12}$	438	2-n-hexylnaphthalene	$C_{16}H_{20}$
394	2-phenyl-1-BUTENE	$C_{10}H_{12}$	439	1-n-heptylnaphthalene	$C_{17}H_{22}$
395	Biphenyl	$C_{12}H_{10}$	440	1-n-octylnaphthalene	$C_{18}H_{24}$
396	1-methyl-2-phenylbenzene	$C_{13}H_{12}$	441	1-N-nonylnaphthalene	$C_{19}H_{26}$
397	1-methyl-3-phenylbenzene	$C_{13}H_{12}$	442	2-N-nonylnaphthalene	$C_{19}H_{26}$
398	1-methyl-4-phenylbenzene	$C_{13}H_{12}$	443	1-N-decylnaphthalene	$C_{20}H_{28}$
399	1-ethyl-4-phenylbenzene	$C_{14}H_{14}$	444	1,2,3,4-tetrahydronaphthalene	$C_{10}H_{12}$
400	1-methyl-4(4-methylphenyl)benzene	$C_{14}H_{14}$	445	1-methyl-[1,2,3,4-tetrahydronaphthalene]	$C_{11}H_{14}$
401	Diphenylmethane	$C_{13}H_{12}$	446	l-ethyl-[1,2,3,4-tetrahydronaphthalene]	$C_{12}H_{16}$
402	1,1-diphenylethane	$C_{14}H_{14}$	447	2,2-dimethyl-[1,2,3,4-tetrahydronaphthalene]	$C_{12}H_{16}$
403	1,2-diphenylethane	$C_{14}H_{14}$	448	2,6-dimethyl-[1,2,3,4-tetrahydronaphtnalene]	$C_{12}H_{16}$
404	1,1-diphenylpropane	$C_{15}H_{16}$	449	6,7-dimethyl-[1,2,3,4-tetrahydronaphthalene]	$C_{12}H_{16}$
405	1,2-diphenylpropane	$C_{15}H_{16}$	450	1-n-propyl-[1,2,3,4-tetrahydronaphthalene]	$C_{13}H_{18}$
406	1,1-dipmenyloutane	$C_{16}H_{18}$	451	6-n-propyl-[1,2,3,4-tetrahydronaphthalene)	$C_{13}H_{18}$
407	1,1-dipmenylpentane	$C_{17}H_{20}$	452	1-n-butyl-[1,2,3,4-tetrahydronaphthalene]	$C_{14}H_{20}$
408	1,1-diphenylhexane	$C_{18}H_{22}$	453	6-n-butyl-[1,2,3,4-tetrahydronaphthalene]	$C_{14}H_{20}$
409	1,1-dipmenylheptane	$C_{19}H_{24}$	454	1-n-pentyl-[1,2,3,4-tetrahydronaphthalene)	$C_{15}H_{22}$
410	1,1-diphenyloctane	$C_{20}H_{26}$	455	6-n-pentyl-[1,2,3,4-tetrahydronaphthaleme]	$C_{15}H_{22}$
411	1,1-diphenylnonane	$C_{21}H_{28}$	456	1-n-hexyl-[1,2,3,4-tetrahydronaphthalene]	$C_{16}H_{24}$
412	1,1-diphenyldecane	$C_{22}H_{30}$	457	1-n-heptyl-[l,2,3,4-tetrahydronaphtnalene]	$C_{17}H_{26}$
413	1,1-dipmenylundecane	$C_{23}H_{32}$	458	1-n-octyl-[1,2,3,4-tetrahydronaphthalene)	$C_{18}H_{28}$
414	1,1-diphenyldodecane	$C_{24}H_{34}$	459	1-n-nonyl-[1,2,3,4-tetrahydronaphthalene)	$C_{19}H_{30}$
415	1,1-diphenyltridecane	$C_{25}H_{36}$	460	1-n-decyl-[1,2,3,4-tetrahydronaphthalene)	$C_{20}H_{32}$
416	1,1-diphenyltetradecane	$C_{26}H_{38}$	461	Indene	C_9H_8
417	1,1-diphenylpentadecane	$C_{27}H_{40}$	462	1-methylindene	$C_{10}H_{10}$
418	Cis-1,2-diphenylethene	$C_{14}H_{12}$	463	2-methylindene	$C_{10}H_{10}$
419	Trans-1,2-dipmenylethene	$C_{14}H_{12}$	464	2,3-dihydroindene	C_9H_{10}
420	Phenylacetylene	C_8H_6	465	1-methyl-2,3-dihydroindene	$C_{10}H_{12}$
421	Diphenylacetylene	$C_{14}H_{10}$	466	2-methyl-2,3-dihydroindene	$C_{10}H_{12}$
422	1,2-diphenylbenzene	$C_{18}H_{14}$	467	4-methyl-2,3-dihydroindene	$C_{10}H_{12}$
423	1,3-diphenylbenzene	$C_{18}H_{14}$	468	5-methyl-2,3-dihydroindene	$C_{10}H_{12}$
424	1,4-diphenylbenzene	$C_{18}H_{14}$	469	Acenaphthalene	$C_{12}H_8$
425	Naphthalene	$C_{10}H_8$	470	Acenaphthene	$C_{12}H_{10}$
426	1-methylnaphthalene	$C_{11}H_{10}$	471	Fluorene	$C_{13}H_{10}$
427	2-methylnaphthalene	$C_{11}H_{10}$	472	Anthracene	$C_{14}H_{10}$
428	1-ethylnaphthalene	$C_{12}H_{12}$	473	Phenanthrene	$C_{14}H_{10}$
429	2-ethylnaphthalene	$C_{12}H_{12}$	474	Pyrene	$C_{16}H_{10}$
430	1,2-dimethylnaphthalene	$C_{12}H_{12}$	475	Fluoranthene	$C_{16}H_{10}$
431	1,4-dimethylnaphthalene	$C_{12}H_{12}$	476	Chrysene	$C_{18}H_{12}$

References

[1] P. Chan, C. Tong, and M. Durrant, *Estimation of boiling points using density functional theory with polarized continuum model solvent corrections*, J Mol Graph Model, 30 (2011), 120–128.

[2] G. S. Cholakov, W. A. Wakeham, and R. P. Stateva, *Estimation of normal boiling points of hydrocarbons from descriptors of molecular structure*, Fluid Phase Equilib, 163 (1999), 21–42.

[3] O. Ivanciuc, T. Ivanciuc, and A. T. Balaban, *Quantitative structure-property relationship study of normal boiling points for halogen-/ oxygen-/ sulfur-containing organic compounds using the codessa program*, Tetrahedron, 54 (1998), 9129–9142.

[4] A. R. Katritzky, L. Mu, V. S. Lobanov, and M. Karelson, *Correlation of boiling points with molecular structure. 1. A training set of 298 diverse organics and a test set of 9 simple inorganics*, J Phys Chem, 100 (1996), 10400–10407.

[5] J. Walker, *The boiling points of homologous compounds. Part I. Simple and mixed ethers*, J Chem Soc Trans, 65 (1894), 193–202.

[6] S. Wang, S.-T. Lin, J. Chang, W. A. Goddard III, and S. I. Sandler, *Application of the COSMO-SAC-BP solvation model to predictions of normal boiling temperatures for environmentally significant substances*, Ind Eng Chem Res, 45 (2006), 5426–5434.