Chapter 12
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Prediction of Critical Temperature and Pressure of Hydrocarbons Using Simple Molecular Properties

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ABSTRACT

Four hundred and seventy (470) hydrocarbons (C_nH_m) were utilized to fit their critical temperature (T_c) and critical pressure (P_c) as functions of molecular weight and carbon atomic fraction. The proposed model is of the form: $T_c=a*(C_{frac})^{b}*(MW)^{c}$ and $P_c= a*(C_{frac})^{1/3}+b*(MW)^{1/3}+c$ 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 $(12n + m)$. The model was found to predict both T_c and P_c with an adequate accuracy, manifested via the associated percent relative error (PRE) of the curve-fitted T_c and P_c. Out of the examined 470 hydrocarbons, low MW compounds were found to have PRE values higher than 10% for the predicted T_c values. On the other hand, for Pc prediction, higher PRE values were found for higher molecular weight compounds, with C_{26} and above.
Although the proposed model does not strictly differentiate among isomers having the same molecular weight and chemical formula, nevertheless, the difference in Tc and Pc among isomers is not significant to be picked up by a simple, straight forward model. A more rigorous model will work hard to offset such small differences in Tc and Pc among isomers, nevertheless, at the expense of model simplicity.

Keywords: Model; critical temperature; critical pressure; hydrocarbons; carbon atoms; molecular formula.

1. INTRODUCTION

The prediction of physicochemical properties like the critical properties of a substance is a major target of computational chemistry. Critical properties are major physicochemical properties used to identify a compound. Critical properties are fundamental characteristics of a chemical compound, and they are 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 priori [1].

Mebane et al. [2] used a simple and convenient method for predicting critical constants (Tc, Pc, and Vc) for members of a homologous series based on computed molecular surface areas obtained from a molecular modeling program (CAChe version 3.5). The best linear correlations were obtained when Vc and $Tc \times Pc^{0.5}$ were plotted against computed molecular surface area (SA) and when Tc and Pc were plotted against the natural logarithm of surface area, ln SA, for 11 homologous series with a total of 118 organic compounds.

Jalowka and Daubert [3] used the group contribution method for predicting critical properties of hydrocarbons using second-order, Benson-type groups. The critical temperature model utilized the normal boiling point and the sub-molecular groups as parameters. On the other hand, the critical pressure model used the normal boiling point, the critical temperature, and the sub-molecular groups as parameters.

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Skander and Chitour [4] used the group-contribution for estimation of the critical properties of 375 pure hydrocarbons using 40 different predictive group contributions. The method was tested with satisfactory accuracy. The absolute average deviations obtained between experimental and calculated values were 0.36%, 4.6%, and 1.7%, respectively, for critical temperature, critical pressure, and critical volume. The proposed equations remained valid in the case of long chain paraffins (up to C40), which was not the case of the majority of other group contribution methods.

Zhiwei et al. [5] used an alternative method based on the linear free energy relationships (LFERs) theory and thermodynamics formulas to predict the critical pressure (Pc) of pure fluids According to their regression results, covering 15 homologues and 516 substances, correlation equations between Pc and molecular descriptors were obtained. The mean relative deviations (MD) of the 15 equations were found to vary from 1.68% to 3.76%. In addition, the squared correlation coefficients (R2) of most of equations were larger than 0.91. Their results revealed that their proposed equations exhibited better effects with a simple form of the equation, high prediction accuracy, definition theory meaning, and wide applicability.

Zuas and Styarini [6] used a quantitative structure-property relationships (QSPR) approach to relate the critical volume (Vc) of unsaturated hydrocarbons, alkenes, and alkynes compounds, to their molecular structures. A QSPR study of Vc was performed based on simple connectivity indices (SCI's). The obtained QSPR model was predictive and required only one SCI descriptor in the calculation with statistical parameters, including standard coefficient correlation (R2) = 0.997, cross-validated correlation coefficients (Q2) = 0.976, and average absolute error (AAE) = 0.12. Application of the best QSPR model to testing a set of 30 alkenes and alkynes demonstrated a good predictability without sufficing any experimental, physicochemical properties.

Sobati and Abooali [7] proposed a quantitative structure–property relationships (QSPR) approach to estimate critical properties of pure refrigerants. For developing these models, the experimental data of TC for 198 pure compounds, the experimental data of VC for 194 pure compounds, and the experimental data of PC for 197 pure compounds were applied. For each compound, 1650 molecular descriptors were determined. Enhanced replacement method (ERM), as an effectual tool for subset variable selection, was utilized. The proposed models were simple multivariate linear equations with six variables for estimation of TC, five variables for estimation of VC, and six variables for estimation of PC. The variables of models were computed from the molecular structure of refrigerants. The average absolute relative deviation (AARD, %) of the proposed models over all experimental data were 2.65%, 3.76%, and 4.65% for estimation of TC, VC, and PC, respectively.

In this model, the critical temperature (Tc) and pressure (Pc) of a hydrocarbon compound is expressed as a function of simple molecular indicators, namely, the carbon atomic fraction (C_{frac}) and molecular weight (*MW*). Such molecular indicators are really simple to calculate. For example, given methane (CH_4), then its C_{frac} will be *1/(1+4)=0.20*. Moreover, its *MW* is simply equal to 1×12+4×1=16. On the other hand, the difference in Tc and Pc among isomers having the same 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 (470) hydrocarbon compounds were used in the non-linear regression process for finding the best fit for their critical 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, & 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, & 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, & ethyl-cyclo-alkene.
7. Alkyne: Contains a $CC{\equiv}CC$ triple bond between carbons. Example: Acetylene, methyl acetylene, pentyne, and hexyne.
8. Aromatic with a single ring: Example: Benzene, toluene, & 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 either the critical temperature (Tc) or critical pressure (Pc) represented the dependent variable (*Z*) from regression point of view:

$$Z = a \times (X)^b \times (Y)^c = Tc\ [K] = a\left(C_{frac}\right)^b \times (MW)^c = \quad (1a)$$

$$Z = a \times (X)^{\frac{1}{3}} + b \times (Y)^{\frac{1}{3}} + c = Pc\ [bar] = a \times \left(C_{frac}\right)^{\frac{1}{3}} + b \times (MW)^{\frac{1}{3}} + c \quad (1b)$$

For example, given methane (*CH4*), then its C_{frac} will be *1/(1+4)=0.20*. Moreover, its *MW* is simply equal to 1×12+4×1=16.

After trying different forms of *Z=f(X,Y)*, the results of non-linear regression for equation (1a), with 95% confidence interval, are:

$$Z = Tc\ [K] = (123.8 \mp 0.9) \times \left(C_{frac}\right)^{(0.229 \pm 0.0021)} \times (MW)^{(0.3577 \pm 0.0015)} \quad (2a)$$

The goodness of fit for Eq. (2a) is given by *R-square* as 0.9986 and adjusted *R-square* as 0.9985 with the sum of squared error (SSE) of 10,155 K^2 and root mean squared error (RMSE) of 4.663 K. The root mean squared error is essentially the standard error in MATLAB® notation.

On the other hand, the regression results of equation (1b), with 95% confidence interval, are:

$$Z = Pc\ [bar] = (37.13 \mp 0.45)\left(C_{frac}\right)^{\frac{1}{3}} - (9.585 \mp 0.047)(MW)^{\frac{1}{3}} + (44.93 \mp 0.41) \quad (2b)$$

The goodness of fit for Eq. (2b) is given by *R-square* as 0.9977 and adjusted *R-square* as 0.9977 with the sum of squared error (SSE) of 80.0 bar^2 and root mean squared error (RMSE) of 0.414 bar.
The percent relative error, PRE is defined as:

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

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

3. RESULTS AND DISCUSSION

For Tc prediction, the mean PRE for all examined compounds was found to be 2.99 % with a standard error of 3.92 %. However, Table 1 shows compounds that have PRE higher than 10%.

Table 1. Small size molecules, like methane, ethylene, and acetylene were found to have highest PRE values for predicting Tc, using Eq. (2a).

Database SN[a]	Compound	Formula	PRE %
1	METHANE	CH4	27.6
94	METHYLCYCLOPROPANE	C4H8	29.2
179	CYCLOOCTANE	C8H16	11.7
180	CYCLONONANE	C9H18	12.6
183	CIS-DECAHYDRONAPHTHALENE	C10H18	10.2
185	1-METHYL-[CIS-DECAHYDRO-NAPHTHALENE]	C11H20	13.7
186	1-METHYL-[TRANS-DECAHYDRO-NAPHTHALENE]	C11H20	12.3
191	ETHYLENE	C2H4	23.3
192	PROPYLENE	C3H6	10.3
289	PROPADIENE	C3H4	10.4
291	1,3-BUTADIENE	C4H6	10.6
303	2-METHYL-1,5-HEXADIENE	C7H12	18.6
304	2-METHYL-2,4-HEXADIENE	C7H12	25.4
305	2,6-OCTADIENE	C8H14	23.4
306	2,6-DIMETHYL-1,5-HEPTADIENE	C9H16	24.7
307	3,7-DIMETHYL-1,6-OCTADIENE	C10H18	25.0
320	ACETYLENE	C2H2	28.8
324	VINYLACETYLENE	C4H4	12.1
414	1,1-DIPHENYLPENTADECANE	C27H40	10.1
415	1,1-DIPHENYLHEXADECANE	C28H42	10.8

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

On the other hand, for Pc prediction, the mean PRE for all examined compounds was found to be 7.73 % with a standard error of 8.7 %. There are 108 compounds with a PRE > 10%. For simplicity, Table 2 shows six compounds with the highest PRE values, being greater than 40%.

Table 2. Large size molecules, (above C26) were found to have PRE higher than 40% for predicting Pc value, using Eq. (2b).

Database SN[a]	Compound	Formula	PRE %
26	N-HEXACOSANE	C26H54	42.1
27	N-HEPTACOSANE	C27H56	49.5
28	N-OCTACOSANE	C28H58	57.3
29	N-NONACOSANE	C29H60	65.5
30	N-TRIACONTANE	C30H62	74.0
177	N-EICOSYLCYCLOHEXANE	C26H52	41.8

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

Other than that, the given two models can predict well Tc and with a reasonable accuracy Pc of a hydrocarbon as a function of its molecular size and carbon atomic (mole) fraction.

Fig. 1 shows the plot of the experimental Tc versus the curve-fitted Tc for all examined 470 hydrocarbons. Most of the data points fall on the 45° diagonal (*Y=X*). There is, however, a small deviation in the high-temperature region. Appendix A contains all hydrocarbons used in this study.

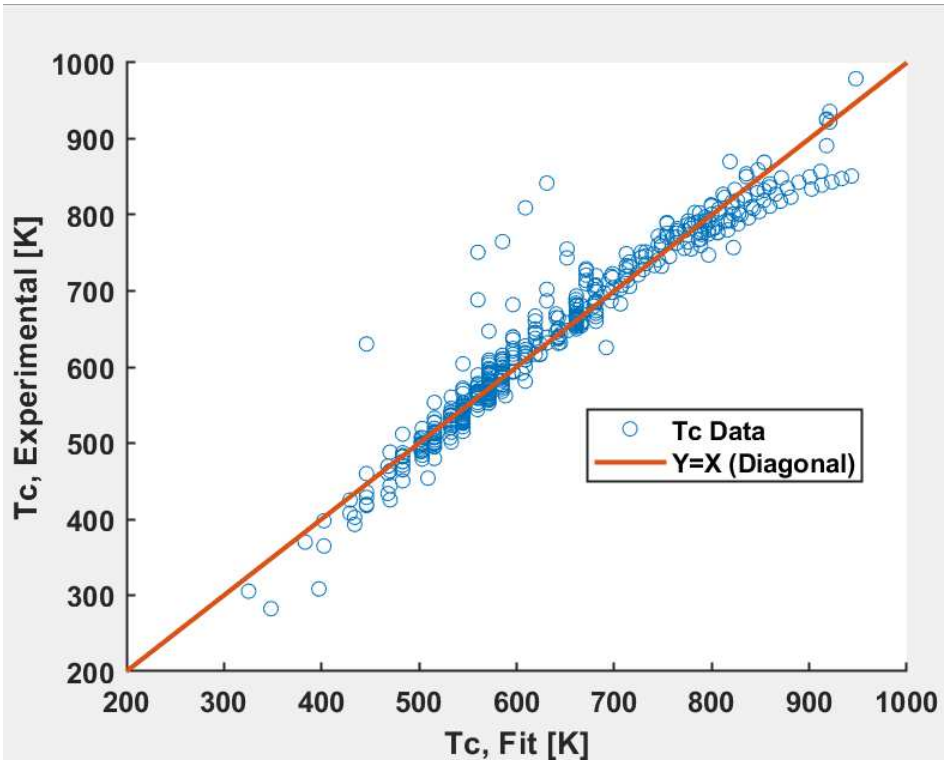

Fig. 1. Plot of experimental Tc versus curve-fitted Tc for all examined 470 hydrocarbons

Fig. 2 shows the plot of the experimental Pc versus the curve-fitted Pc for all examined 470 hydrocarbons. Most of the data points fall on the 45° diagonal (Y=X). There is, however, a small deviation both in the low- and high-pressure region.

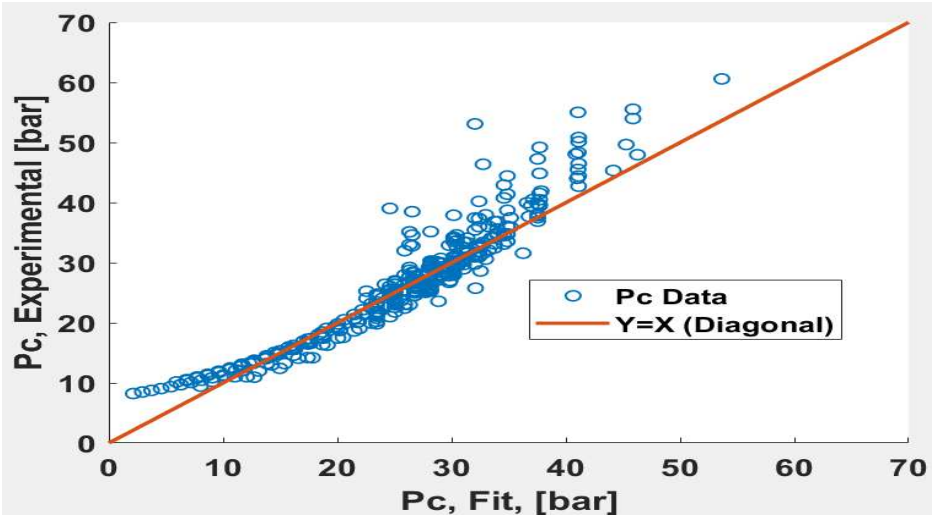

Fig. 2. Plot of experimental Pc versus curve-fitted Pc for all examined 470 hydrocarbons

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

Table 3. Eighteen different stereo chemical compounds with the same molecular weight (114.3) and same chemical formula (C_8H_{18})

SN[a]	Compound	Tc, K	Pc, bar
8	N-OCTANE	568.9	24.54
46	2-METHYLHEPTANE	559.6	24.52
47	3-METHYLHEPTANE	563.7	25.13
48	4-METHYLHEPTANE	561.7	25.07
49	3-ETHYLHEXANE	565.4	25.76
50	2,2-DIMETHYLHEXANE	549.8	24.97
51	2,3-DIMETHYLHEXANE	563.4	25.96
52	2,4-DIMETHYLHEXANE	553.5	25.27
53	2,5-DIMETHYLHEXANE	550.0	24.57
54	3,3-DIMETHYLHEXANE	562.0	26.15
55	3,4-DIMETHYLHEXANE	568.8	26.55
56	2-METHYL-3-ETHYLPENTANE	567.0	26.65
57	3-METHYL-3-ETHYLPENTANE	576.5	27.73
58	2,2,3-TRIMETHYLPENTANE	563.5	26.94
59	2,2,4-TRIMETHYLPENTANE	544.0	25.34
60	2,3,3-TRIMETHYLPENTANE	573.5	27.83
61	2,3,4-TRIMETHYLPENTANE	566.3	26.94
62	2,2,3,3-TETRAMETHYLBUTANE	567.8	28.32

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

Based on the proposed model (Eq. 2a), the predicted Tc is:

$$Tc = (123.8) \times (0.30769)^{(0.229)} \times (114.23)^{(0.3577)} = 514.7\ K$$

On the other hand, the predicted Pc is given by Eq. (2b) as:

$$Pc = (37.13)(0.30769)^{\frac{1}{3}} - (9.585)(114.23)^{\frac{1}{3}} + (44.93) = 23.49\ bar$$

Table 4 shows the minimum, maximum, and the mean value of both Tc and Pc for different isomers of C_8H_{18} compound as well as its predicted Tc and Pc value.

Table 4. The minimum, maximum, and the mean Tc and Pc of isomers of C_8H_{18} compound, shown in Table 3.

	Tc, K	Predicted Tc	PRE (%)	Pc	Predicted Pc	PRE (%)
Minimum	544.0	514.7	5.4	24.52	23.49	4.2
Maximum	576.5	514.7	10.7	28.32	23.49	17.0
Mean	562.5	514.7	8.5	26.01	23.49	9.7

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

For such a set of stereo-chemical compounds, the value given for Tc by Eq. (2a) matches the mean value shown in Table 4, with a PRE value of 8.5%. On the other hand, the value given for Pc by Eq. (2b) matches the mean value shown in Table 4, with a PRE value of 9.7%.

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, the difference in Tc and Pc

for the same set of stereo chemical isomers falls within 10% PRE value. A more rigorous model will work hard to offset this 10 % PRE value, but at the expense of model simplicity.

4. CONCLUSION

The Tc and Pc for a hydrocarbon compound could be expressed as a function of simple molecular properties with an adequate accuracy manifested via the associated percent relative error (PRE) of the curve-fitted Tc and Pc. 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 470 hydrocarbons, low molecular weight compounds were found to have PRE values higher than 10% for predicting Tc. On the other hand, the maximum deviation between given and predicted value of Pc occurs at higher molecular weights, with C26 and above.

COMPETING INTERESTS

Author has declared that no competing interests exist.

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APPENDIX A

List of 470 hydrocarbons used in the non-linear regression process to express Tc and Pc as a function of hydrocarbon molecular weight and its carbon atomic fraction:

SN	Compound	Formula	C#	H#	MW	Tc	Pc
1	METHANE	CH4	1	4	16.04	190.5	45.3
2	ETHANE	C2H6	2	6	30.07	305.3	48.07
3	PROPANE	C3H8	3	8	44.10	369.8	41.92
4	N-BUTANE	C4H10	4	10	58.12	425.2	37.47
5	N-PENTANE	C5H12	5	12	72.15	469.7	33.25
6	N-HEXANE	C6H14	6	14	86.18	507.4	29.73
7	N-HEPTANE	C7H16	7	16	100.2	540.2	27.00
8	N-OCTANE	C8H18	8	18	114.2	568.8	24.54
9	N-NONANE	C9H20	9	20	128.3	594.6	22.58
10	N-DECANE	C10H22	10	22	142.3	617.6	20.77
11	N-UNDECANE	C11H24	11	24	156.3	639.1	19.05
12	N-DODECANE	C12H26	12	26	170.3	658.4	17.57
13	N-TRIDECANE	C13H28	13	28	184.4	676.1	16.28
14	N-TETRADECANE	C14H30	14	30	198.4	696.8	14.19
15	N-PENTADECANE	C15H32	15	32	212.4	707.3	14.11
16	N-HEXADECANE	C16H34	16	34	226.4	721.2	13.22
17	N-HEPTADECANE	C17H36	17	36	240.5	733.4	13.00
18	N-OCTADECANE	C18H38	18	38	254.5	745.3	11.98
19	N-NONADECANE	C19H40	19	40	268.5	755.9	11.02
20	N-EICOSANE	C20H42	20	42	282.5	767.0	11.02
21	N-HENEICOSANE	C21H44	21	44	296.6	781.7	11.32
22	N-DOCOSANE	C22H46	22	46	310.6	791.8	10.87
23	N-TRICOSANE	C23H48	23	48	324.6	801.3	10.45
24	N-TETRACOSANE	C24H50	24	50	338.7	810.3	10.06
25	N-PENTACOSANE	C25H52	25	52	352.7	818.9	9.70
26	N-HEXACOSANE	C26H54	26	54	366.7	827.2	9.37
27	N-HEPTACOSANE	C27H56	27	56	380.7	835.2	9.06
28	N-OCTACOSANE	C28H58	28	58	394.8	842.8	8.76
29	N-NONACOSANE	C29H60	29	60	408.8	850.0	8.49
30	N-TRIACONTANE	C30H62	30	62	422.8	857.2	8.23
31	ISOBUTANE	C4H10	4	10	58.1	407.8	35.90
32	ISOPENTANE	C5H12	5	12	72.1	460.4	33.40
33	NEOPENTANE	C5H12	5	12	72.15	433.8	31.60
34	2-METHYLPENTANE	C6H14	6	14	86.18	497.5	29.71
35	3-METHYLPENTANE	C6H14	6	14	86.18	504.4	30.83
36	2,2-DIMETHYLBUTANE	C6H14	6	14	86.18	488.8	30.40
37	2,3-DIMETHYLBUTANE	C6H14	6	14	86.18	500.0	30.86
38	2-METHYLHEXANE	C7H16	7	16	100.2	530.4	26.98
39	3-METHYLHEXANE	C7H16	7	16	100.2	535.2	27.77
40	3-ETHYLPENTANE	C7H16	7	16	100.2	540.6	28.53
41	2,2-DIMETHYLPENTANE	C7H16	7	16	100.2	520.5	27.37
42	2,3-DIMETHYLPENTANE	C7H16	7	16	100.2	537.3	28.70
43	2,4-DIMETHYLPENTANE	C7H16	7	16	100.2	519.8	27.01
44	3,3-DIMETMYLPENTANE	C7H16	7	16	100.2	536.4	29.07
45	2,2,3-TRIMETHYLBUTANE	C7H16	7	16	100.2	531.2	29.15

SN	Compound	Formula	C#	H#	MW	Tc	Pc
46	2-METHYLHEPTANE	C8H18	8	18	114.2	559.6	24.52
47	3-METHYLHEPTANE	C8H18	8	18	114.2	563.7	25.13
48	4-METHYLHEPTANE	C8H18	8	18	114.2	561.7	25.07
49	3-ETHYLHEXANE	C8H18	8	18	114.2	565.4	25.76
50	2,2-DIMETHYLHEXANE	C8H18	8	18	114.2	549.8	24.97
51	2,3-DIMETHYLHEXANE	C8H18	8	18	114.2	563.4	25.96
52	2,4-DIMETHYLHEXANE	C8H18	8	18	114.2	553.5	25.27
53	2,5-DIMETHYLHEXANE	C8H18	8	18	114.2	550.0	24.57
54	3,3-DIMETHYLHEXANE	C8H18	8	18	114.2	562.0	26.15
55	3,4-DIMETHYLHEXANE	C8H18	8	18	114.2	568.8	26.55
56	2-METHYL-3-ETHYLPENTANE	C8H18	8	18	114.2	567.0	26.65
57	3-METHYL-3-ETHYLPENTANE	C8H18	8	18	114.2	576.5	27.73
58	2,2,3-TRIMETHYLPENTANE	C8H18	8	18	114.2	563.5	26.94
59	2,2,4-TRIMETHYLPENTANE	C8H18	8	18	114.2	544.0	25.34
60	2,3,3-TRIMETHYLPENTANE	C8H18	8	18	114.2	573.5	27.83
61	2,3,4-TRIMETHYLPENTANE	C8H18	8	18	114.2	566.3	26.94
62	2,2,3,3-TETRAMETHYLBUTANE	C8H18	8	18	114.2	567.8	28.32
63	2-METHYLOCTANE	C9H20	9	20	128.3	586.7	22.60
64	3-METHYLOCTANE	C9H20	9	20	128.3	590.1	23.10
65	4-METHYLOCTANE	C9H20	9	20	128.3	587.6	23.10
66	3-ETHYLHEPTANE	C9H20	9	20	128.3	594.3	23.98
67	2,2-DIMETHYLHEPTANE	C9H20	9	20	128.3	577.5	23.06
68	2,6-DIMETHYLHEPTANE	C9H20	9	20	128.3	576.6	21.81
69	2,2,3-TRIMETHYLHEXANE	C9H20	9	20	128.3	591.3	25.07
70	2,2,4-TRIMETHYLHEXANE	C9H20	9	20	128.3	574.2	23.39
71	2,2,5-TRIMETHYLHEXANE	C9H20	9	20	128.3	568.05	23.00
72	2,3,3-TRIMETHYLHEXANE	C9H20	9	20	128.3	599.3	25.56
73	2,3,5-TRIMETHYLHEXANE	C9H20	9	20	128.3	582.6	23.49
74	2,4,4-TRIMETHYLHEXANE	C9H20	9	20	128.3	582.2	23.78
75	3,3,4-TRIMETHYLHEXANE	C9H20	9	20	128.3	603.7	26.45
76	3,3-DIETHYLPENTANE	C9H20	9	20	128.3	610.05	26.40
77	2,2-DIMETHYL-3-ETHYLPENTANE	C9H20	9	20	128.3	589.6	25.39
78	2,4-DIMETHYL-3-ETHYLPENTANE	C9H20	9	20	128.3	590.9	24.98
79	2,2,3,3-TETRAMETHYLPENTANE	C9H20	9	20	128.3	610.8	27.00
80	2,2,3,4-TETRAMETHYLPENTANE	C9H20	9	20	128.3	592.1	25.30
81	2,2,4,4-TETRAMETHYLPENTANE	C9H20	9	20	128.3	571.3	23.30
82	2,3,3,4-TETRAMETHYLPENTANE	C9H20	9	20	128.3	607.6	26.84
83	2-METHYLNONANE	C10H22	10	22	142.3	609.3	20.23
84	3-METHYLNONANE	C10H22	10	22	142.3	613.7	21.12
85	4-METHYLNONANE	C10H22	10	22	142.3	619.0	21.82
86	5-METHYLNONANE	C10H22	10	22	142.3	609.7	21.31
87	2,7-DIMETHYLOCTANE	C10H22	10	22	142.3	600.5	19.84
88	3,3,4-TRIMETHYLHEPTANE	C10H22	10	22	142.3	627.7	24.48
89	3,3,5-TRIMETHYLHEPTANE	C10H22	10	22	142.3	609.6	22.90
90	2,2,3,3-TETRAMETHYLHEXANE	C10H22	10	22	142.3	623.0	24.77
91	2,2,5,5-TETRAMETHYLHEXANE	C10H22	10	22	142.3	581.4	21.61
92	2,4-DIMETHYL-3-ISOPROPYL-PENTANE	C10H22	10	22	142.3	614.4	23.49
93	CYCLOPROPANE	C3H6	3	6	42.1	397.9	55.02

SN	Compound	Formula	C#	H#	MW	Tc	Pc
94	METHYLCYCLOPROPANE	C4H8	4	8	56.1	630.3	44.86
95	ETHYLCYCLOPROPANE	C5H10	5	10	70.1	481.9	38.72
96	CIS-1,2-DIMETHYLCYCLOPROPANE	C5H10	5	10	70.1	483.7	38.72
97	CYCLOBUTANE	C4H8	4	8	56.1	459.9	49.20
98	METHYLCYCLOBUTANE	C5H10	5	10	70.1	487.3	41.40
99	ETHYLCYCLOBUTANE	C6H12	6	12	84.2	526.8	36.00
100	CYCLOPENTANE	C5H10	5	10	70.1	511.8	44.43
101	METHYLCYCLOPENTANE	C6H12	6	12	84.2	532.8	37.35
102	ETHYLCYCLOPENTANE	C7H14	7	14	98.2	569.5	33.53
103	1,1-DIMETHYLCYCLOPENTANE	C7H14	7	14	98.2	547.0	34.02
104	CIS-1,2-DIMETHYLCYCLOPENTANE	C7H14	7	14	98.2	565.1	34.00
105	TRANS-1,2-DIMETHYLCYCLOPENTANE	C7H14	7	14	98.2	553.1	34.00
106	CIS-1,3-DIMETHYLCYCLOPENTANE	C7H14	7	14	98.2	550.9	34.02
107	TRANS-1,3-DIMETHYLCYCLOPENTANE	C7H14	7	14	98.2	553.1	34.02
108	N-PROPYLCYCLOPENTANE	C8H16	8	16	112.2	603	29.61
109	ISOPROPYLCYCLOPENTANE	C8H16	8	16	112.2	593.2	30.01
110	1-METHYL-1-ETHYLCYCLOPENTANE	C8H16	8	16	112.2	582.1	29.82
111	CIS-l-METHYL-2-ETHYL-CYCLOPENTANE	C8H16	8	16	112.2	591.7	29.82
112	TRANS-l-METHYL-2-ETHYL-CYCLOPENTANE	C8H16	8	16	112.2	581.6	29.82
113	CIS-l-METHYL-3-ETHYL-CYCLOPENTANE	C8H16	8	16	112.2	581.5	29.82
114	TRANS-1-METHYL-3-ETHYL-CYCLOPENTANE	C8H16	8	16	112.2	581.5	29.82
115	1,1,2-TRIMETMYLCYCLOPENTANE	C8H16	8	16	112.2	570.6	29.82
116	1,1,3-TRIMETMYLCYCLOPENTANE	C8H16	8	16	112.2	557.5	29.82
117	l,CIS-2,CIS-3-TRIMETHYL-CYCLOPENTANE	C8H16	8	16	112.2	584.3	29.82
118	l,CIS-2,TRANS-3-TRIMETHYL-CYCLOPENTANE	C8H16	8	16	112.2	576.1	29.82
119	l,TRANS-2,CIS-3-TRIMETHYL-CYCLOPENTANE	C8H16	8	16	112.2	565.7	29.82
120	l,CIS-2,CIS-4-TRIMETHYL-CYCLOPENTANE	C8H16	8	16	112.2	575.0	29.82
121	l,CIS-2,TRANS-4-TRIMETMYL-CYCLOPENTANE	C8H16	8	16	112.2	576.1	29.82
122	l,TRANS-2,CIS-4-TRIMETHYL-CYCLOPENTANE	C8H16	8	16	112.2	564.0	29.82
123	N-BUTYLCYCLOPENTANE	C9H18	9	18	126.2	621.3	26.88
124	ISOBUTYLCYCLOPENTANE	C9H18	9	18	126.2	624.3	28.74
125	1-METHYL-1-n-PROPYL- CYCLOPENTANE	C9H18	9	18	126.2	605.9	26.88
126	1,1-DIETHYLCYCLOPENTANE	C9H18	9	18	126.2	612.4	26.88
127	CIS-1,2-DIETHYLCYCLOPENTANE	C9H18	9	18	126.2	616.9	26.88
128	1,1-DIMETHYL-2-ETHYL-CYCLOPENTANE	C9H18	9	18	126.2	594.4	26.88
129	N-PENTYLCYCLOPENTANE	C10H20	10	20	140.3	644.1	24.46

SN	Compound	Formula	C#	H#	MW	Tc	Pc
130	N-HEXYLCYCLOPENTANE	C11H22	11	22	154.3	665.0	22.44
131	N-HEPTYLCYCLOPENTANE	C12H24	12	24	168.3	684.0	20.73
132	N-OCTYLCYCLOPENTANE	C13H26	13	26	182.3	701.4	19.26
133	N-NONYLCYCLOPENTANE	C14H28	14	28	196.4	717.5	17.98
134	N-DECYLCYCLOPENTANE	C15H30	15	30	210.4	732.4	16.86
135	N-UNDECYLCYCLOPENTANE	C16H32	16	32	224.4	746.2	15.88
136	N-OODECYLCYCLOPENTANE	C17H34	17	34	238.5	758.9	15.00
137	N-TRIDECYLCYCLOPENTANE	C18H36	18	36	252.5	770.9	14.21
138	N-TETRADECYLCYCLOPENTANE	C19H38	19	38	266.5	782.3	13.51
139	N-PENTADECYLCYCLOPENTANE	C20H40	20	40	280.5	792.6	12.87
140	N-HEXADECYLCYCLOPENTANE	C21H42	21	42	294.6	803.0	12.28
141	N-HEPTADECYLCYCLOPENTANE	C22H44	22	44	308.6	811.2	11.75
142	N-OCTADECYLCYCLOPENTANE	C23H46	23	46	322.6	820.7	11.26
143	N-NONADECYLCYCLOPENTANE	C24H48	24	48	336.6	829.2	10.81
144	N-EICOSYLCYCLOPENTANE	C25H50	25	50	350.7	836.6	10.40
145	CYCLOHEXANE	C6H12	6	12	84.2	553.5	40.22
146	METHYLCYCLOHEXANE	C7H14	7	14	98.2	572.2	34.26
147	ETHYLCYCLOHEXANE	C8H16	8	16	112.2	609.1	30.00
148	1,1-DIMETHYLCYCLOHEXANE	C8H16	8	16	112.2	591.1	29.00
149	CIS-1,2-DIMETHYLCYCLOHEXANE	C8H16	8	16	112.2	606.1	29.00
150	TRANS-1,2-DIMETHYLCYCLOHEXANE	C8H16	8	16	112.2	596.1	29.00
151	CIS-I,3-DIMETMYLCYCLOHEXANE	C8H16	8	16	112.2	591.1	29.00
152	TRANS-1,3-DIMETHYLCYCLOHEXANE	C8H16	8	16	112.2	598.1	29.00
153	CIS-I,4-DIMETHYLCYCLOHEXANE	C8H16	8	16	112.2	598.1	29.00
154	TRANS-1,4-DIMETHYLCYCLOHEXANE	C8H16	8	16	112.2	590.1	29.00
155	N-PROPYLCYCLOHEXANE	C9H18	9	18	126.2	639.1	27.70
156	ISOPROPYLCYCLOHEXANE	C9H18	9	18	126.2	635.9	35.14
157	N-BUTYLCYCLOHEXANE	C10H20	10	20	140.3	667.0	25.36
158	ISOBUTYLCYCLOHEXANE	C10H20	10	20	140.3	660.4	39.04
159	SEC-BUTYLCYCLOHEXANE	C10H20	10	20	140.3	649.9	25.52
160	TERT-BUTYLCYCLOHEXANE	C10H20	10	20	140.3	645.6	26.06
161	1-METHYL-4-ISOPROPYL- CYCLOHEXANE	C10H20	10	20	140.3	637.6	25.52
162	N-PENTYLCYCLOHEXANE	C11H22	11	22	154.3	669.7	23.22
163	N-HEXYLCYCLOHEXANE	C12H24	12	24	168.3	688.6	21.39
164	N-HEPTYLCYCLOHEXANE	C13H26	13	26	182.3	706.6	19.82
165	N-OCTYLCYCLOHEXANE	C14H28	14	28	196.4	722.7	18.47
166	N-NONYLCYCLOHEXANE	C15H30	15	30	210.4	738.1	17.29
167	N-DECYLCYCLOHEXAME	C16H32	16	32	224.4	751.2	16.26
168	N-UNDECYLCYCLOHEXANE	C17H34	17	34	238.5	764.0	15.34
169	N-DODECYLCYCLOHEXANE	C18H36	18	36	252.5	775.9	14.52
170	N-TRIDECYLCYCLOHEXANE	C19H38	19	38	266.5	787.0	13.78
171	N-TETRADECYLCYCLOHEXANE	C20H40	20	40	280.5	797.3	13.11
172	N-PENTADECYLCYCLOHEXANE	C21H42	21	42	294.6	807.6	12.51
173	N-HEXADECYLCYCLOHEXANE	C22H44	22	44	308.6	816.8	11.96
174	N-MEPTADECYLCYCLOHEXANE	C23H46	23	46	322.6	825.0	11.45
175	N-OCTADECYLCYCLOHEXANE	C24H48	24	48	336.6	833.4	10.99
176	N-NONADECYLCYCLOHEXANE	C25H50	25	50	350.7	840.7	10.56
177	N-EICOSYLCYCLOHEXANE	C26H52	26	52	364.7	848.6	10.16
178	CYCLOHEPTANE	C7H14	7	14	98.2	604.3	37.90

SN	Compound	Formula	C#	H#	MW	Tc	Pc
179	CYCLOOCTANE	C8H16	8	16	112.2	647.1	35.18
180	CYCLONONANE	C9H18	9	18	126.2	682.0	33.00
181	ETHYLCYCLOHEPTANE	C9H18	9	18	126.2	639.7	29.22
182	BICYCLOHEXYL	C12H22	12	22	166.3	727	25.27
183	CIS-DECAHYDRONAPHTHALENE	C10H18	10	18	138.2	702.25	32.00
184	TRANS-DECAHYDRONAPHTMALENE	C10H18	10	18	138.2	687.05	28.00
185	1-METHYL-[CIS-DECAHYDRO-NAPHTHALENE]	C11H20	11	20	152.3	755.1	26.42
186	1-METHYL-[TRANS-DECAHYDRO-NAPHTHALENE]	C11H20	11	20	152.3	743.4	26.42
187	1-ETHYL-[CIS-DECAHYDRO- NAPHTHALENE]	C12H22	12	22	166.3	729.3	24.08
188	1-ETHYL-[TRANS-DECAHYDRO-NAPHTHALENE]	C12H22	12	22	166.3	713.7	24.08
189	9-ETHYL-[CIS-DECAHYDRONAPHTHALENE]	C12H22	12	22	166.3	720.8	24.08
190	9-ETHYL-[TRANS-DECAHYDRO-NAPHTHALENE]	C12H22	12	22	166.3	709.4	24.08
191	ETHYLENE	C2H4	2	4	28.0	282.4	49.66
192	PROPYLENE	C3H6	3	6	42.1	364.8	45.52
193	1-BUTENE	C4H8	4	8	56.1	419.6	39.67
194	CIS-2-BUTENE	C4H8	4	8	56.1	435.6	41.51
195	TRANS-2-BUTENE	C4H8	4	8	56.1	428.6	40.49
196	ISOBUTENE	C4H8	4	8	56.1	417.9	39.47
197	1-PENTENE	C5H10	5	10	70.1	464.8	34.80
198	CIS-2-PENTENE	C5H10	5	10	70.1	475.9	36.06
199	TRANS-2-PENTENE	C5H10	5	10	70.1	475.4	36.06
200	2-METHYL-1-BUTENE	C5H10	5	10	70.1	465.4	33.55
201	3-METHYL-1-BUTENE	C5H10	5	10	70.1	450.4	34.70
202	2-METHYL-2-BUTENE	C5H10	5	10	70.1	470.9	33.55
203	1-HEXENE	C6H12	6	12	84.2	503.7	30.99
204	CIS-2-HEXENE	C6H12	6	12	84.2	513.0	31.19
205	TRANS-2-HEXENE	C6H12	6	12	84.2	513.0	31.19
206	CIS-3-HEXENE	C6H12	6	12	84.2	507.7	31.26
207	TRANS-3-HEXENE	C6H12	6	12	84.2	508.5	31.26
208	2-METHYL-1-PENTENE	C6H12	6	12	84.2	507.0	31.19
209	3-METHYL-1-PENTENE	C6H12	6	12	84.2	494.8	32.53
210	4-METHYL-1-PENTENE	C6H12	6	12	84.2	496.0	31.78
211	2-METHYL-2-PENTENE	C6H12	6	12	84.2	514.0	31.19
212	CIS-3-METHYL-2-PENTENE	C6H12	6	12	84.2	515.3	32.53
213	TRANS-3-METHYL-2-PENTENE	C6H12	6	12	84.2	519.4	32.53
214	CIS-4-METHYL-2-PENTENE	C6H12	6	12	84.2	499.0	31.78
215	TRANS-4-METHYL-2-PENTENE	C6H12	6	12	84.2	501.0	31.78
216	2-ETHYL-1-BUTENE	C6H12	6	12	84.2	512.0	31.19
217	2,3-DIMETHYL-1-BUTENE	C6H12	6	12	84.2	500.0	31.78
218	3,3-DIMETHYL-1-BUTENE	C6H12	6	12	84.2	479.9	32.44
219	2,3-DIMETHYL-2-BUTENE	C6H12	6	12	84.2	527.6	32.77
220	1-HEPTENE	C7H14	7	14	98.2	537.4	27.93
221	CIS-2-HEPTENE	C7H14	7	14	98.2	549	28.03
222	TRANS-2-HEPTENE	C7H14	7	14	98.2	543.1	28.13

SN	Compound	Formula	C#	H#	MW	Tc	Pc
223	CIS-3-HEPTENE	C7H14	7	14	98.2	545.0	28.03
224	TRANS-3-HEPTENE	C7H14	7	14	98.2	539.7	28.13
225	2-METHYL-1-HEXENE	C7H14	7	14	98.2	537.8	28.31
226	3-METHYL-1-HEXENE	C7H14	7	14	98.2	527.7	29.13
227	4-METHYL-1-HEXENE	C7H14	7	14	98.2	531.9	29.13
228	5-METHYL-1-HEXENE	C7H14	7	14	98.2	527.9	28.31
229	2-METHYL-2-HEXENE	C7H14	7	14	98.2	542.8	28.31
230	CIS-3-METHYL-2-HEXENE	C7H14	7	14	98.2	547.52	29.13
231	TRANS-3-METHYL-2-HEXENE	C7H14	7	14	98.2	544.4	29.13
232	CIS-4-METHYL-2-HEXENE	C7H14	7	14	98.2	531.3	29.13
233	TRANS-4-METHYL-2-HEXENE	C7H14	7	14	98.2	533.1	29.13
234	CIS-5-METHYL-2-HEXENE	C7H14	7	14	98.2	534.1	28.31
235	TRANS-5-METHYL-2-HEXENE	C7H14	7	14	98.2	532.1	28.31
236	TRANS-2-METHYL-3-HEXENE	C7H14	7	14	98.2	529.0	28.31
237	TRANS-2-METHYL-3-HEXENE	C7H14	7	14	98.2	528.8	28.31
238	CIS-3-METHYL-3-HEXENE	C7H14	7	14	98.2	544.722	29.13
239	TRANS-3-METHYL-3-HEXENE	C7H14	7	14	98.2	542.0	29.13
240	2-ETHYL-1-PENTENE	C7H14	7	14	98.2	542.7	29.13
241	3-ETHYL-1-PENTENE	C7H14	7	14	98.2	529.9	29.97
242	3-ETHYL-2-PENTENE	C7H14	7	14	98.2	547.6	29.97
243	2,3-DIMETHYL-1-PENTENE	C7H14	7	14	98.2	533.8	30.18
244	2,4-DIMETHYL-1-PENTENE	C7H14	7	14	98.2	526.0	28.50
245	3,3-DIMETHYL-1-PENTENE	C7H14	7	14	98.2	526.6	30.79
246	3,4-DIMETHYL-1-PENTENE	C7H14	7	14	98.2	528.6	30.18
247	4,4-DIMETHYL-1-PENTENE	C7H14	7	14	98.2	515.3	29.06
248	2,3-DIMETHYL-2-PENTENE	C7H14	7	14	98.2	553.4	30.18
249	2,4-DIMETHYL-2-PENTENE	C7H14	7	14	98.2	528.5	28.50
250	CIS-3,4-DIMETHYL-2-PENTENE	C7H14	7	14	98.2	541.3	30.18
251	TRANS-3,4-DIMETHYL-2-PENTENE	C7H14	7	14	98.2	544.6	30.18
252	CIS-4,4-DIMETHYL-2-PENTENE	C7H14	7	14	98.2	527.1	29.06
253	TRANS-4,4-DIMETHYL-2-PENTENE	C7H14	7	14	98.2	521.6	29.06
254	3-METHYL-2-ETHYL-1-BUTEME	C7H14	7	14	98.2	535.0	29.32
255	2,3,3-TRIMETHYL-1-BUTENE	C7H14	7	14	98.2	531.1	31.00
256	1-OCTENE	C8H16	8	16	112.2	567.0	25.27
257	TRANS-2-OCTENE	C8H16	8	16	112.2	572.5	25.55
258	TRANS-2-OCTENE	C8H16	8	16	112.2	577.0	25.46
259	TRANS-3-OCTENE	C8H16	8	16	112.2	568.5	25.55
260	TRANS-3-OCTENE	C8H16	8	16	112.2	574.0	25.46
261	TRANS-4-OCTENE	C8H16	8	16	112.2	568.0	25.55
262	TRANS-4-OCTENE	C8H16	8	16	112.2	573.0	25.46
263	2-METHYL-1-HEPTENE	C8H16	8	16	112.2	563.4	25.55
264	3-METHYL-1-HEPTENE	C8H16	8	16	112.2	556.4	26.35
265	4-METHYL-1-HEPTENE	C8H16	8	16	112.2	559.0	26.35
266	TRANS-6-METMYL-2-HEPTENE	C8H16	8	16	112.2	563.3	25.70
267	TRANS-3-METHYL-3-HEPTENE	C8H16	8	16	112.2	570.9	26.35
268	2-ETHYL-1-HEXENE	C8H16	8	16	112.2	574.0	30.30
269	3-ETHYL-1-HEXENE	C8H16	8	16	112.2	557.2	27.03
270	4-ETHYL-1-HEXENE	C8H16	8	16	112.2	561.1	27.03
271	2,3-DIMETHYL-1-HEXENE	C8H16	8	16	112.2	560.9	27.19

SN	Compound	Formula	C#	H#	MW	Tc	Pc
272	2,3-DIMETHYL-2-HEXENE	C8H16	8	16	112.2	577.4	27.19
273	CIS-2,2-DIMETHYL-3-HEXENE	C8H16	8	16	112.2	552.6	26.30
274	2,3,3-TRIMETHYL-1-PENTENE	C8H16	8	16	112.2	568.4	29.37
275	2,4,4-TRIMETHYL-1-PENTENE	C8H16	8	16	112.2	553.0	25.96
276	2,4,4-TRIMETHYL-2-PENTENE	C8H16	8	16	112.2	558.0	25.96
277	1-NONENE	C9H18	9	18	126.2	593.2	23.00
278	1-DECENE	C10H20	10	20	140.3	616.8	21.02
279	1-UNDECENE	C11H22	11	22	154.3	646.0	19.94
280	1-DODECENE	C12H24	12	24	168.3	666.0	18.65
281	1-TRIDECENE	C13H26	13	26	182.3	685.0	17.47
282	1-TETRADECENE	C14H28	14	28	196.4	704.0	16.38
283	1-PENTADECENE	C15H30	15	30	210.4	705.9	14.21
284	1-HEXADECENE	C16H32	16	32	224.4	736.0	14.61
285	1-HEPTADECENE	C17H34	17	34	238.5	732.4	12.44
286	1-OCTADECENE	C18H36	18	36	252.5	763.0	13.22
287	1-NONADECENE	C19H38	19	38	266.5	755.1	10.95
288	1-EICOSENE	C20H40	20	40	280.5	788.0	12.04
289	PROPADIENE	C3H4	3	4	40.1	393.1	53.98
290	1,2-BUTADIENE	C4H6	4	6	54.1	444.0	44.41
291	1,3-BUTADIENE	C4H6	4	6	54.1	425.4	42.73
292	1,2-PENTADIENE	C5H8	5	8	68.1	491.6	37.50
293	CIS-1,3-PENTAOrENE	C5H8	5	8	68.1	499.0	36.91
294	TRANS-1,3-PENTADIENE	C5H8	5	8	68.1	500.0	36.91
295	1,4-PENTADIENE	C5H8	5	8	68.1	479.0	36.91
296	2,3-PENTADIENE	C5H8	5	8	68.1	496.9	37.50
297	3-METHYL-1,2-BUTADIENE	C5H8	5	8	68.1	489.5	37.83
298	2-METHYL-1,3-BUTADIENE	C5H8	5	8	68.1	484.0	38.00
299	1,2-HEXADIENE	C6H10	6	10	82.1	526.4	33.10
300	1,5-HEXADIENE	C6H10	6	10	82.1	501.4	33.10
301	2,3-HEXADIENE	C6H10	6	10	82.1	514.3	33.10
302	3-METHYL-1,2-PENTADIENE	C6H10	6	10	82.1	523.4	34.50
303	2-METHYL-1,5-HEXADIENE	C7H12	7	12	96.2	688.3	29.79
304	2-METHYL-2,4-HEXADIENE	C7H12	7	12	96.2	750.8	29.79
305	2,6-OCTADIENE	C8H14	8	14	110.2	764.9	26.73
306	2,6-DIMETHYL-1,5-HEPTADIENE	C9H16	9	16	124.2	809.2	25.22
307	3,7-DIMETHYL-1,6-OCTADIENE	C10H18	10	18	138.2	841.8	23.09
308	CYCLOPENTENE	C5H8	5	8	68.1	507.0	47.27
309	1-METHYL-CYCLOPENTENE	C6H10	6	10	82.1	545.6	40.78
310	1-ETHYLCYCLOPENTENE	C7H12	7	12	96.2	578.4	35.46
311	3-ETHYLCYCLOPENTENE	C7H12	7	12	96.2	578.4	53.10
312	1-N-PROPYLCYCLOPENTENE	C8H14	8	14	110.2	600.1	28.96
313	CYCLOHEXENE	C6H10	6	10	82.1	560.4	42.93
314	1-METHYLCYCLOHEXENE	C7H12	7	12	96.2	589.6	37.45
315	1-ETHYLCYCLOHEXENE	C8H14	8	14	110.2	615.4	32.91
316	CYCLOPENTADIENE	C5H6	5	6	66.1	507.0	50.83
317	DICYCLOPENTADIENE	C10H12	10	12	132.2	660.0	30.20
318	ALPHA-PINENE	C10H16	10	16	136.2	632.0	27.24
319	BETA-PINENE	C10H16	10	16	136.2	643.0	27.24
320	ACETYLENE	C2H2	2	2	26.0	308.3	60.59

SN	Compound	Formula	C#	H#	MW	Tc	Pc
321	METHYLACETYLENE	C3H4	3	4	40.1	402.4	55.54
322	DIMETHYLACETYLENE	C4H6	4	6	54.1	488.1	50.14
323	ETHYLACETYLENE	C4H6	4	6	54.1	463.6	46.48
324	VINYLACETYLENE	C4H4	4	4	52.1	454.0	47.96
325	1-PENTYNE	C5H8	5	8	68.1	494.2	39.84
326	2-PENTYNE	C5H8	5	8	68.1	519.3	39.84
327	1-HEXYNE	C6H10	6	10	82.1	528.7	34.86
328	1-HEPTYNE	C7H12	7	12	96.2	558.6	30.96
329	1-OCTYNE	C8H14	8	14	110.2	585.4	27.83
330	1-NOMYNE	C9H16	9	16	124.2	609.4	25.26
331	1-DECYNE	C10H18	10	18	138.2	631.8	22.45
332	BENZENE	C6H6	6	6	78.1	562.2	48.34
333	TOLUENE	C7H8	7	8	92.1	591.8	40.55
334	ETHYLBENZENE	C8H10	8	10	106.2	617.2	35.62
335	O-XYLENE	C8H10	8	10	106.2	630.4	36.85
336	M-XYLENE	C8H10	8	10	106.2	617.0	34.95
337	P-XYLENE	C8H10	8	10	106.2	616.3	34.65
338	N-PROPYLBENZENE	C9H12	9	12	120.2	638.4	31.58
339	ISOPROPYLBENZENE	C9H12	9	12	120.2	631.1	31.67
340	O-ETHYLTOLUENE	C9H12	9	12	120.2	651.1	33.34
341	M-ETHYLTOLUENE	C9H12	9	12	120.2	637.1	32.05
342	P-ETHYLTOLUENE	C9H12	9	12	120.2	640.1	31.91
343	1,2,3-TRIMETHYLBENZENE	C9H12	9	12	120.2	664.5	34.09
344	1,2,4-TRIMETHYLBENZENE	C9H12	9	12	120.2	649.1	31.90
345	1,3,5-TRIMETHYLBENZENE	C9H12	9	12	120.2	637.4	30.86
346	N-BUTYLBENZENE	C10H14	10	14	134.2	660.5	28.49
347	ISOBUTYLBENZENE	C10H14	10	14	134.2	650.1	30.00
348	SEC-BUTYLBENZENE	C10H14	10	14	134.2	664.5	29.12
349	TERT-BUTYLBENZENE	C10H14	10	14	134.2	660.0	29.31
350	1-METHYL-2-N-PROPYLBENZENE	C10H14	10	14	134.2	662.4	29.01
351	1-METHYL-3-N-PROPYLBENZENE	C10H14	10	14	134.2	654.6	27.70
352	1-METMYL-4-N-PROPYLBENZENE	C10H14	10	14	134.2	656.6	27.70
353	O-CYMENE	C10H14	10	14	134.2	662.0	28.92
354	M-CYMENE	C10H14	10	14	134.2	657.0	28.92
355	P-CYNENE	C10H14	10	14	134.2	653.1	28.00
356	O-DIETHYLBENZENE	C10H14	10	14	134.2	668.0	28.42
357	M-DIETHYLBENZENE	C10H14	10	14	134.2	663.0	28.42
358	P-DIETHYLBENZENE	C10H14	10	14	134.2	658.0	27.66
359	1,2-DIMETHYL-3-ETHYLBENZENE	C10H14	10	14	134.2	680.0	28.42
360	1,2-DIMETHYL-4-ETHYLBENZENE	C10H14	10	14	134.2	666.3	28.47
361	1,3-DIMETHYL-2-ETHYLBENZENE	C10H14	10	14	134.2	670.7	29.84
362	1,3-DIMETHYL-4-ETHYLBENZENE	C10H14	10	14	134.2	664.4	28.47
363	1,3-DIMETHYL-5-ETHYLBENZENE	C10H14	10	14	134.2	665.4	29.84
364	1,4-DIMETHYL-2-ETHYLBENZENE	C10H14	10	14	134.2	670.7	28.47
365	1,2,3,4-TETRAMETHYLBENZENE	C10H14	10	14	134.2	693.4	30.71
366	1,2,3,5-TETRAMETHYLBENZENE	C10H14	10	14	134.2	681.4	29.28
367	1,2,4,5-TETRAMETHYLBENZENE	C10H14	10	14	134.2	675.1	29.00
368	N-PENTYLBENZENE	C11H16	11	16	148.2	679.9	25.72
369	N-HEXYLBENZENE	C12H18	12	18	162.3	698.0	23.49

SN	Compound	Formula	C#	H#	MW	Tc	Pc
370	N-HEPTYLBENZENE	C13H20	13	20	176.3	713.5	21.71
371	N-OCTYLBENZENE	C14H22	14	22	190.3	728.1	20.07
372	N-NONYLBENZENE	C15H24	15	24	204.4	740.9	18.71
373	N-DECYLBENZENE	C16H26	16	26	218.4	771.0	17.47
374	N-UNDECYLBENZENE	C17H28	17	28	232.4	764.3	16.47
375	N-DODECYLBENZENE	C18H30	18	30	246.4	774.3	15.58
376	N-TRIDECYLBENZENE	C19H32	19	32	260.5	783.0	14.80
377	N-TETRADECYLBENZENE	C20H34	20	34	274.5	792.0	14.02
378	N-PENTADECYLBENZENE	C21H36	21	36	288.5	800.4	13.27
379	N-HEXADECYLBENZENE	C22H38	22	38	302.5	808.1	12.72
380	CYCLOHEXYLBENZENE	C12H16	12	16	160.3	733.0	28.42
381	STYRENE	C8H8	8	8	104.1	648.0	39.48
382	CIS-l-PROPENYL BENZENE	C9H10	9	10	118.2	654.0	33.14
383	TRANS-l-PROPENYL BENZENE	C9H10	9	10	118.2	670.1	33.14
384	2-PROPENYL BENZENE	C9H10	9	10	118.2	657.0	33.16
385	1-METHYL-2-ETHENYL BENZENE	C9H10	9	10	118.2	658.6	34.23
386	1-METHYL-3-ETHENYL BENZENE	C9H10	9	10	118.2	657.1	32.44
387	1-METHYL-4-ETHENYL BENZENE	C9H10	9	10	118.2	658.9	32.44
388	1-METHYL-4-(TRANS-1-N-PROPENYL)BENZENE	C10H12	10	12	132.2	686.6	28.98
389	1-ETHYL-2-ETHENYL BENZENE	C10H12	10	12	132.2	670.5	30.39
390	l-ETHYL-3-ETHENYL BENZENE	C10H12	10	12	132.2	670.6	28.98
391	l-ETHYL-4-ETHENYL BENZENE	C10H12	10	12	132.2	674.0	28.98
392	2-PHENYL-1-BUTENE	C10H12	10	12	132.2	666.3	29.70
393	BIPHENYL	C12H10	12	10	154.2	789.3	37.97
394	1-METHYL-2-PHENYLBENZENE	C13H12	13	12	168.2	759.6	29.24
395	1-METHYL-3-PHENYLBENZENE	C13H12	13	12	168.2	780.5	28.05
396	1-METHYL-4-PHENYLBENZENE	C13H12	13	12	168.2	776.7	28.05
397	1-ETHYL-4-PHENYLBENZENE	C14H14	14	14	182.3	747.2	25.44
398	1-METHYL-4(4-METHYLPHENYL)-BENZENE	C14H14	14	14	182.3	793.1	25.06
399	DIPHENYLMETHANE	C13H12	13	12	168.2	768.0	28.82
400	1,1-DIPHENYLETHANE	C14H14	14	14	182.3	775.0	26.45
401	1,2-DIPHENYLETHANE	C14H14	14	14	182.3	780.0	26.15
402	1,1-DIPHENYLPROPANE	C15H16	15	16	196.3	776.4	23.70
403	1,2-DIPHENYLPROPANE	C15H16	15	16	196.3	777.0	23.70
404	1,1-DIPMENYLOUTANE	C16H18	16	18	210.3	780.2	21.81
405	1,1-DIPMENYLPENTANE	C17H20	17	20	224.3	788.2	20.20
406	1,1-DIPHENYLHEXANE	C18H22	18	22	238.4	796.1	18.81
407	1,1-DIPMENYLHEPTANE	C19H24	19	24	252.4	804.2	17.59
408	1,1-DIPHENYLOCTANE	C20H26	20	26	266.4	811.5	16.52
409	1,1-DIPHENYLNONANE	C21H28	21	28	280.4	817.9	15.58
410	1,1-DIPHENYLDECANE	C22H30	22	30	294.5	823.3	14.74
411	1,1-DIPHENYLDODECANE	C24H34	24	34	322.5	833.9	13.30
412	1,1-DIPHENYLTRIDECANE	C25H36	25	36	336.6	839.1	12.15
413	1,1-DIPHENYLTETRADECANE	C26H38	26	38	350.6	843.2	11.14
414	1,1-DIPHENYLPENTADECANE	C27H40	27	40	364.6	847.6	10.26
415	1,1-DIPHENYLHEXADECANE	C28H42	28	42	378.6	851.0	9.47
416	CIS-1,2-DIPHENYLETHENE	C14H12	14	12	180.2	757.0	27.04

SN	Compound	Formula	C#	H#	MW	Tc	Pc
417	TRANS-1,2-DIPMENYLETHENE	C14H12	14	12	180.2	801.0	27.04
418	PHENYLACETYLENE	C8H6	8	6	102.1	625.5	44.03
419	DIPHENYLACETYLENE	C14H10	14	10	178.2	832.0	28.62
420	1,2-DIPHENYLBENZENE	C18H14	18	14	230.3	890.9	38.50
421	1,3-DIPHENYLBENZENE	C18H14	18	14	230.3	924.8	34.60
422	1,4-DIPHENYLBENZENE	C18H14	18	14	230.3	925.9	32.80
423	NAPHTHALENE	C10H8	10	8	128.2	748.3	39.98
424	1-METHYLNAPHTHALENE	C11H10	11	10	142.2	772.0	36.02
425	2-METHYLNAPHTHALENE	C11H10	11	10	142.2	761.0	32.07
426	1-ETHYLNAPHTHALENE	C12H12	12	12	156.2	775.7	32.74
427	2-ETHYLNAPHTHALENE	C12H12	12	12	156.2	770.7	31.28
428	1,2-DIMETHYLNAPHTHALENE	C12H12	12	12	156.2	788.5	33.67
429	1,4-DIMETHYLNAPHTHALENE	C12H12	12	12	156.2	789.9	34.63
430	1-N-PROPYLNAPHTHALENE	C13H14	13	14	170.2	781.8	29.27
431	2-N-PROPYLNAPHTHALENE	C13H14	13	14	170.2	778.9	28.08
432	1-N-BUTYLNAPHTHALENE	C14H16	14	16	184.3	792.0	26.45
433	2-N-BUTYLNAPHTHALENE	C14H16	14	16	184.3	787.7	25.47
434	1-N-PENTYLNAPHTHALENE	C15H18	15	18	198.3	802.8	24.13
435	1-N-HEXYLNAPHTHALENE	C16H20	16	20	212.3	813.3	22.18
436	2-N-HEXYLNAPHTHALENE	C16H20	16	20	212.3	811.5	21.47
437	1-N-HEPTYLNAPHTHALENE	C17H22	17	22	226.4	827.1	20.51
438	1-N-OCTYLNAPHTHALENE	C18H24	18	24	240.4	833.3	19.08
439	1-N-NONYLNAPHTHALENE	C19H26	19	26	254.4	854.0	16.58
440	2-N-NONYLNAPHTHALENE	C19H26	19	26	254.4	850.2	17.37
441	1-N-DECYLNAPHTHALENE	C20H28	20	28	268.4	859.0	15.59
442	1,2,3,4-TETRAHYDRONAPHTHALENE	C10H12	10	12	132.2	720.1	32.57
443	1-METHYL-[1,2,3,4-TETRAHYDRONAPHTHALENE]	C11H14	11	14	146.2	719.4	30.17
444	l-ETHYL-[1,2,3,4-TETRAHYDRONAPHTHALENE]	C12H16	12	16	160.3	733.1	27.16
445	2,2-DIMETHYL-[1,2,3,4-TETRAHYDRONAPHTHALENE]	C12H16	12	16	160.3	719.5	27.16
446	2,6-DIMETHYL-[1,2,3,4-TETRAHYDRONAPHTNALENE]	C12H16	12	16	160.3	728.1	26.72
447	6,7-DIMETHYL-[1,2,3,4-TETRAHYDRONAPHTHALENE]	C12H16	12	16	160.3	749.0	27.39
448	1-N-PROPYL-[1,2,3,4-TETRAHYDRONAPHTHALENE]	C13H18	13	18	174.3	744.5	24.70
449	6-N-PROPYL-[1,2,3,4-TETRAHYDRONAPHTHALENE)	C13H18	13	18	174.3	751.1	24.33
450	1-N-HEXYL-[1,2,3,4-TETRAHYDRONAPHTHALENE]	C16H24	16	24	216.4	779.0	19.41
451	1-N-HEPTYL-[l,2,3,4-TETRAHYDRONAPHTNALENE]	C17H26	17	26	230.4	791.1	18.11
452	1-N-OCTYL-[1,2,3,4-TETRAHYDRONAPHTHALENE)	C18H28	18	28	244.4	801.0	16.98
453	1-N-NONYL-[1,2,3,4-TETRAHYDRONAPHTHALENE)	C19H30	19	30	258.4	822.9	15.98
454	1-N-DECYL-[1,2,3,4-	C20H32	20	32	272.5	819.0	15.09

SN	Compound	Formula	C#	H#	MW	Tc	Pc
	TETRAHYDRONAPHTHALENE)						
455	INDENE	C9H8	9	8	116.2	687.0	37.70
456	1-METHYLINDENE	C10H10	10	10	130.2	703.1	34.14
457	2-METHYLINDENE	C10H10	10	10	130.2	682.9	34.14
458	2,3-DIHYDROINDENE	C9H10	9	10	118.2	681.1	36.85
459	1-METHYL-2,3-DIHYDROINDENE	C10H12	10	12	132.2	684.8	32.46
460	2-METHYL-2,3-DIHYDROINDENE	C10H12	10	12	132.2	686.0	32.46
461	4-METHYL-2,3-DIHYDROINDENE	C10H12	10	12	132.2	707.9	33.45
462	5-METHYL-2,3-DIHYDROINDENE	C10H12	10	12	132.2	698.7	31.82
463	ACENAPHTHALENE	C12H8	12	8	152.2	792.0	31.58
464	ACENAPHTHENE	C12H10	12	10	154.2	803.1	30.59
465	FLUORENE	C13H10	13	10	166.2	870.0	46.39
466	ANTHRACENE	C14H10	14	10	178.2	869.0	32.96
467	PHENANTHRENE	C14H10	14	10	178.2	869.2	28.62
468	PYRENE	C16H10	16	10	202.2	936.0	25.76
469	FLUORANTHENE	C16H10	16	10	202.2	922.0	25.76
470	CHRYSENE	C18H12	18	12	228.3	979.0	23.59

Biography of author(s)

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A portable, platform-independent professor of chemical engineering is currently mounted at Higher Colleges of Technology, UAE. He holds B.S., M.S., and Ph.D. degrees all in chemical/biochemical engineering. He graduated from Oregon State University in 1993, and his area of specialty during M.S. and Ph.D. programs dealt with protein interactions and behaviour at interfaces in biological systems. He currently researches in the modelling, simulation, and optimization aspects of physical/biophysical systems and characterization of molecular properties within the dome of chemical, biochemical, pharmaceutical, and food engineering. He is a sole book author with renowned publishers: Al-Malah, K., "Aspen Plus: Chemical Engineering Applications", Wiley & Sons, Inc. and Al-Malah, K., "MATLAB®: Numerical Methods with Chemical Engineering Applications", McGraw Hill, Inc. In addition to his traditional and classical field of study, he is a software developer, using Microsoft Visual Studio technology, and has created a bundle of Windows-based or MATLAB-based software for engineering applications (https://sites.google.com/view/al-malah/software).
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