## ORIGINAL PAPER

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# **Reparameterized Austin Model 1 for quantitative structure-property relationships in liquid media**

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Abstract A reparameterization of the quantum-chemical AM1 (Austin Model 1) model has been carried out using a nonlinear optimization based on a modification of the Levenberg-Marquardt technique. The optimum numerical values for the one-electron resonance integral parameters  $(\beta_s \text{ and } \beta_n)$  and core-core repulsion atomic parameters  $\alpha$ were obtained for the elements H, C, N, O, Cl and Br using the statistical fit of a two-parameter QSPR equation for the boiling points of organic compounds. A substantially improved two-parameter correlation ( $R^2$ =0.9685, s=13.48 K) was obtained by using the new optimized parameters. The QSPR equation employs two molecular descriptors, a bulk cohesiveness descriptor,  $\sqrt[3]{G_I}$  and the area-weighted surface charge of hydrogen-bonding donor atom(s) in the molecule. The model developed shows remarkably accurate predictions of the normal boiling points for nine additional simple inorganic compounds. The new parameters were tested on the critical temperatures of 165 organic compounds. The new QSPR model obtained for this property was found to be statistically significantly better than the original model.

**Keywords** Semiempirical parameterization · QSPR · Boiling point · Critical temperature

#### Introduction

Quantum-chemical molecular descriptors have been widely used in the development of quantitative structureactivity/property relationships (QSAR/QSPR) [1–4]. In most cases, especially when large data sets of relatively large molecules are considered, the descriptors are calculated from the molecular wave function obtained at the semiempirical level of theory. The most common semiempirical parameterizations used are Austin Model 1 (AM1) [5] and Parametric Model 3 (PM3) [6]. These parameterizations were developed by fitting the data on the properties of isolated molecules or those in the gas phase (heats of formation, ionization energies, dipole moments etc.). However, most of the QSPR/QSAR models are built on the data on molecular properties in condensed media (liquids, solutions, and membranes). Indeed, a large variety of quantum chemical models have been developed both at the semiempirical and ab initio level to account for the perturbation of the molecular wave function of a solute in condensed media [7-14]. Unfortunately, these models have only seldom found use in the calculation of molecular descriptors in the liquid phase [15-20]. Therefore, in the present work we wish to examine if a simple reparameterization of the AM1 model could improve the representation of OSPR models for molecular properties in the liquid phase. As a model process for this reparameterization, we have chosen the boiling points of compounds.

First of all, the normal boiling points of compounds provide valuable information in a variety of practical applications [21]. This property has also been applied in various areas of both chemistry and engineering as a powerful parameter that could be used to predict a number of key physical and physicochemical properties. On the other hand, the relationship of the boiling points to the molecular structure, and therefore the molecular properties, is predetermined by the intermolecular interaction in the liquid and by the difference in the molecular internal partition function in the gas phase and in the liquid at the boiling temperature. Our study is based on previously reported results by Katritzky et al. for the boiling points of 298 diverse organic and nine inorganic compounds [22]. Using only a two-descriptor equation, a very significant QSPR model was developed by them for a set of structurally very variable compounds (squared correlation coefficient  $R^2$ =0.954 and standard deviation s=16.15 K). The

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two descriptors used in this model were Eq. (1) (1) the cubic root of the gravitation index  $\sqrt[3]{G_I}$  and (2) the charged surface area of hydrogen-donor atoms *HDSA(2)* [23].

$$T_{b} = (-170.7 \pm 7.46) + (65.88 \pm 0.86) \sqrt[3]{G_{I}} + (18470 \pm 540) HDSA(2)$$
(1)

Mathematically, these descriptors are defined as follows:

$$G_{\rm I} = \sum_{ij} \left( m_i \cdot m_j / r_{ij}^2 \right) \tag{2}$$

where the sum is over *i* and *j* for all bonded pairs of atoms in the molecule,  $m_i$  and  $m_j$  are the atomic masses and  $r_{ij}$  the distance between the *i*-th and *j*-th atoms, and

$$HDSA(2) = \sum \frac{q_D \sqrt{S_D}}{S_{tot}}$$
(3)

where  $q_D$  is the partial charge on hydrogen-bonding donor (H) atom(s),  $S_D$  labels the surface are for this atom, and  $S_{tot}$ is the total molecular surface area, calculated from the van der Waals radii of atoms (overlapping spheres). In the last formula Eq. (3), the summation goes over the number of simultaneously possible hydrogen-bonding donor pairs per molecule. The results obtained in the original article using the CODESSA program [24] showed a strong orthogonality of these descriptors (the pair correlation coefficient between  $\sqrt[3]{G_I}$  and HDSA(2) is only 0.2041). From the physical point of view, both descriptors have obvious meaning;  $G_I$  is connected with the dispersion and cavityformation effects in liquid, HDSA(2) reflects the hydrogenbonding ability of compounds. The theory of condensed media assumes that the energy of cavity formation is proportional to the surface of the molecular cavity. The latter depends on the geometry of the molecule and will thus be directly related to the gravitation index  $G_{I}$ . The second descriptor, HDSA(2) is related to the energy of hydrogen bond formation.

The goal of the present work was to adjust the quantumchemical parameterization for the AM1 semiempirical model to improve the QSPR models of molecular properties in the liquid phase. In general, the new set of semiempirical parameters should produce more adequate characteristics (bond lengths and angles, charges, dipole moments etc.) of the molecules in the liquid phase by using a nonlinear optimization for the AM1(Austin Model) semiempirical parameters  $\alpha$ ,  $\beta_s$  and  $\beta_p$  where  $\alpha$ is core–core repulsion atomic parameter and  $\beta_s$ ,  $\beta_p$ –one– electron resonance integral parameters (for s and p states, respectively) [5], a new set of 17 parameters for the atoms H, C, N, O, Cl and Br (Table 1) were derived. The applicability of the new set of parameters was examined using the QSPR model for the critical temperatures of compounds [25].

Table 1 The original and new optimized AM1 parameters

No	Atom	Parameter	Original values ([5])	Re-optimized values
1	Н	$\alpha$ , Å <sup>-1</sup>	2.882324	2.858038
2	С	$\alpha \text{ Å}^{-1}$	2.648274	2.644260
3	Ν	$\alpha \text{ Å}^{-1}$	2.947286	2.911589
4	0	$\alpha \text{ Å}^{-1}$	4.455371	3.847456
5	Cl	$\alpha \text{ Å}^{-1}$	2.919368	4.428944
6	Br	$\alpha \text{ Å}^{-1}$	2.576546	2.631694
7	Н	$\beta_s$ , eV	-6.173790	-6.236430
8	С	$\beta_s$ , eV	-15.71580	-15.479268
9	Ν	$\beta_s$ , eV	-20.29910	-19.73390
10	0	$\beta_s$ , eV	-29.27280	-27.79330
11	Cl	$\beta_s$ , eV	-24.59470	-25.04320
12	Br	$\beta_s$ , eV	-19.39990	-22.20060
13	С	$\beta_p$ , eV	-7.719280	-7.86513
14	Ν	$\beta_p$ , eV	-18.23870	-19.36820
15	0	$\beta_p$ , eV	-29.27280	-28.05140
16	Cl	$\beta_p$ , eV	-14.63720	-22.78330
17	Br	$\beta_p$ , eV	-8.95720	-8.70759

#### Methodology and optimization

The original set of AM1 parameters was produced by optimization of several properties of the molecules (e.g. bonds, angles, heat of formation etc.). Two kinds of parameter were considered in our reparameterization procedure (Table 1). First, within the AM1 and MNDO<sup>26</sup> formalism, the Fock matrix elements  $F\rho\sigma$  are expressed as follows:

$$F_{\rho\sigma} = \beta_{\rho\sigma} - \frac{1}{2} \sum_{\kappa} \sum_{\lambda} P_{\kappa\lambda} < \rho\kappa | \sigma\lambda >.$$
(4)

where  $\langle \rho \kappa | \sigma \lambda \rangle$  are the two-center two-electron repulsion integrals and  $\beta_{\rho\sigma}$  denote the two-center one-electron core resonance integrals. The latter are approximated to be proportional to the corresponding overlap integrals  $S_{\rho\sigma}$  and a function with an implicit dependence on the interatomic distance  $f_{\rm res}$  ( $R_{AB}$ ) [26]:

$$\beta_{\rho\sigma} = f_{res} \left( R_{AB} \right) S_{\rho\sigma} \tag{5}$$

In MNDO and AM1 models, the function  $f_{\text{res}}$  ( $R_{\text{AB}}$ ) is approximated by:

$$f_{res}(R_{AB}) = (\beta_{\rho}^{A} + \beta_{\sigma}^{B})/2$$
(6)

where  $\beta_{\rho}^{A}$ ,  $\beta_{\rho}^{B}$  are adjustable atomic semiempirical resonance parameters. There exist at most two different  $\beta$  parameters for any first-row element i.e.  $\beta_{s}^{A}$  and  $\beta_{p}^{A}$ , for *s* and *p* AO's, respectively.

As a successor of MNDO [26], AM1 has different parameterization for the core – core repulsion function (CRF) in order to compensate the excessive repulsion due to atom

interactions at van der Waals distance. It is defined as follows

$$CRF(AB) = Z_{A}Z_{B}\gamma_{AB} \{1 + exp(-\alpha_{A}R_{AB}) + exp(-\alpha_{B}R_{AB}) + R_{AB}^{-1}\sum_{i} K_{Ai} exp[L_{Ai}(R_{AB} - M_{Ai})] + R_{AB}^{-1}\sum_{j} K_{Bj} exp[L_{Bj}(R_{AB} - M_{Bj})]\}$$
(7)

where the parameters L determine the width of the Gaussians and M and K are adjustable parameters for the excessive repulsion between atoms at larger van der Waals distances [5]. As seen from Eq. (7), the parameter  $\alpha$  is directly connected to the interatomic interactions, controlling the appropriate behavior of these repulsions with respect to the interatomic distances RAB. Through the above approximations for the electron energy and core-core repulsion energy, the total energy of the molecule can be presented as the parametric function of interatomic distances RAB. In this way, all characteristics of the compounds are calculated at the equilibrium geometry for a given parameterization. Therefore, both  $\alpha$  and  $\beta$  parameters were chosen as arguments in our quantum-chemical reparameterization. The optimization of these parameters thus leads to new equilibrium geometries of molecules at which the new values of molecular descriptors (HDSA(2) and  $G_1$ ) will be calculated that would be more adequate for the QSPR model of boiling points.

The set of 298 molecules is structurally sufficiently diverse and includes saturated hydrocarbons, halogenated compounds, and cyano, ester, ether, hydroxyl, amino, carbonyl and carboxyl functionalities. The critical temperatures of 165 organic compounds from the DIPPR database were the same as in the original work [25]. Most of the compounds had the same chemical functionalities and some of them are overlapped with the set of boiling points. The initial geometry of all compounds was optimized using the MOPAC program [27] with the original semiempirical AM1 parameterization. The molecular descriptors were calculated within the CODESSA PRO software [28].

Considering the overall number of parameters optimized (17), the problem of finding the new AM1 parameters was reduced to finding a minimum of the function  $F(\alpha, \beta_s, \beta_p)$  in 17-dimensional space formed by  $\alpha, \beta_s$  and  $\beta_p$  where *F* is

$$F(\alpha, \beta_{s}, \beta_{p}) = \sum_{k=1}^{298} F_{k}^{2} = \sum_{k=1}^{298} \left( T_{exp}^{k} - T_{calc}^{k} \right)^{2}$$
(8)

where  $T_{exp}^k$  denote experimental boiling points and  $T_{exp}^k$  T are

$$T_{calc}^{k} = X_{1} + X_{2}\sqrt[3]{G_{I}} + X_{3}HDSA(2)$$
(9)

the calculated boiling points ( $X_i$  are coefficients for QSPR

equation).  $F_k$  is thus the difference between the experimental and predicted boiling points for a given ( $\kappa$ th) compound. Because of the nature of the task, the most appropriate approach to solve it can be based on an iterative procedure. We have used a modification of the Levenberg-Marquardt technique [29] to minimize the sum of the squares of nonlinear functions  $F_k$ . Our procedure requires the values for the derivatives of the function being minimized with respect to all variables (Jacobian matrix). The main difficult for the task is the calculation of the derivatives. In the present situation, derivatives of F were found by finite differences. Because of the complexity of the 17-dimensional surface Eq. (8), care should be taken in the calculation of the Jacobian matrix in order to find the right direction that proceeds to the minimum. As initial guess for the parameters  $\alpha$ ,  $\beta_s$  and  $\beta_p$ , the original AM1 parameters [5] were chosen (Table 1). As mentioned above, the structure of molecules was initially optimized with these parameters. In this way, each iteration started with the same geometry of the compounds, but with a different set of  $\alpha$  and  $\beta$  values. At each iteration, with different parameters loaded within MOPAC, the new descriptors ( $G_I$ and HDSA(2)) were calculated by CODESSA-PRO. The latter automatically generates the new QSPR equation with its statistical characteristics ( $X_i$  coefficients of Eq. (9), correlation coefficient  $R^2$ , standard deviation s, t-test etc.) of the model and the predicted boiling points  $T_{\text{calc}}$ . The standard deviation of the QSPR model was chosen as the main optimization criterion for the optimization.

#### **Results and discussion**

The optimization according to Eq. (8) resulted in a new set of AM1 (AM1-BP) parameters shown in Table 1. Notably, there is significant difference in  $\alpha$  parameter for oxygen and chlorine atoms as compared with the original parameters by Dewar et al. [5] The remaining parameters  $\alpha$  were much less changed. The new  $\beta$  parameter values for H and C atoms are close to the original data. A large difference in  $\beta_p$  values was found for chlorine atoms. For the oxygen atom, the values for  $\beta_s$  and  $\beta_p$  were set equal to each other in the original work [5]. However, in our case, these parameters are different. The variance in the parameterization of O and Cl as compared to the original parameters indicates the higher electronegativity of these atoms with respect to the electrostatic molecular interactions in solutesolvent (solute-solute) systems. Thus, this tendency of new optimized AM1 parameters reflects adequately the intermolecular interactions in liquid phase. The statistical characteristics of the final QSPR equation for  $T_b$  is shown in Table 2 (see also Fig. 1 and Table 3 for the predictions). As a rule, the large-sized compounds possess higher boiling temperature. For hydrocarbons, the results of QSPR are very close to the experimental boiling points. This observation indicates that the gravitation index  $G_I$  that accounts simultaneously for both the atomic masses (volumes) and for their distribution within the molecular space describes correctly the dispersion forces and cavity

**Table 2** The QSPR equation for the boiling points (nine), using the descriptors calculated using new AM1 parameterization ( $R^2$ =0.968, s=13.48 K, F=4529.94)

n	Descriptor	$X + \Delta X$	<i>t</i> -test
1 2	Intercept $G_{t}^{1/3}$	-178.66±6.20 66.83±0.72	-28.79 92.60
3	HDSA(2)	19608.05±454.27	43.16

formation processes in the liquid. In general, the larger molecular masses lead to stronger dispersion forces and therefore higher boiling points. These forces also depend on the shape of the molecule, being most important for non-polar species. The energy of cavity formation for a compound is roughly proportional to the molecular volume of the solute, or to the surface area of cavity, and to the microscopic surface tension on the boundary between the solute cavity and the solvent.

The HDSA(2) descriptor combines the surface areas and partial charges of the atoms and successfully addresses the dipole–dipole attractions and hydrogen bonding in liquids. This is also in agreement with the concept that strong dipole–dipole interactions for the formation of hydrogen bonds contribute to the one of the main terms in solvation energy of a molecule [7]. The HDSA(2) descriptor also elucidates the accessibility of the heteroatoms to play an important role in determining the tendency of a molecule to enter the vapor phase.

The optimized semiempirical parameters and the corresponding QSPR model (Eq. (9) and Table 2) were tested on the prediction of the boiling points for a set of nine inorganic compounds (Table 4). Notably, the predictions were significantly better than reported earlier using the descriptors developed from the original AM1 parameterization (average deviation 17 vs. 22 K in the original work).

Another test of the new AM1 parameterization was carried out by the re-development of the earlier QSPR model for the critical temperatures of 165 organic compounds [25]. The new parameters were set up for the MOPAC program and its output files were loaded in CODESSA. Thus, the new molecular descriptors were calculated proceeding from the new geometries and wave functions of the molecules. The new best two-parameter QSPR equation for the critical temperatures found by CODESSA (Table 5), was statistically significantly better than the best two-descriptor equation in the original work [25] ( $R^2$ =0.868, s=28.7 K, F=546). The original model has the same functional dependence on the descriptors as (Table 5). Notably, instead of HDSA(2) descriptor, a similar HASA(2) descriptor was used in the best equation for the critical temperatures (Table 5). Consequently, the AM1 reparameterization also improves the representation of other electrostatic descriptors for the molecules in the liquid phase. All calculated 165 critical temperatures using equation in Table 5 are shown in Table 6 and plotted against the experimental values in Fig. 2.



Fig. 1 The calculated vs experimental normal boiling points according to the best twodescriptor equation (Table 2) and new AM1 parameters

 Table 3 Experimental boiling points vs. calculated boiling points (equation of Table 2) for 298 organic compounds

No.         Compound $T_{un}$ , K $T_{un}$ , K         fst         2.6-xylend         47.422         485.65           1         1.1.dichlaropropane         361.25         370.60         55         2.bromobutane         304.17         304.15           3         1.2.3.4-tertahydromphulene         480.77         460.98         57         2-ethylburyric acid         460.97         400.98         57         2-ethylburyric acid         460.97         400.98         57         2-ethylburyric acid         460.97         400.98         57         2-ethylburyric acid         460.97         400.85         420.76         59         2-ethylburyric acid         480.77         304.38         334.45         376.66         1         2-ethylbornopane         373.78         473.15         506.49           1         1.3-bytotacheadiene         286.77         461.55         32.66         2-ethylboryleneadiene         400.85         403.59           1         1.3-bytotacheadiene         353.49         351.43         65         2-methyl-betanen         301.40           1         1.3-bytotacheadiene         353.15         463.23         70         2-methyl-betanen         312.45         301.40           1         1.3-bytotacheadiene         353.15	(equa	tion of Table 2) for 298 organic co	mpounds		– No	Compound	$T_{\rm exp},  {\rm K}$	$T_{\text{cale}}, \mathbf{K}$
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	No	Compound	$T_{\rm exp},  {\rm K}$	$T_{\text{calc}}, \mathbf{K}$	- 54	2 6-xylenol	474 22	485.65
2         1.1-diphenylethane         545.78         534.34         56         Bromopropane         332.56         335.11           3         1.2,3-4-ternshydromphulene         480.77         400.98         57         2-ethylburytic scid         460.65         480.82           5         1.2,4-trinnethylbenzene         442.53         429.76         59         2-ethyl-1-buttene         337.82         334.28           7         1.2-diphonylethane         535.65         534.66         61         2-thylhexyl acrylate         489.15         506.49           8         1.2-prophylethane         253.65         741.65         62         2-bexamol         401.85         403.90           9         1.3-butakiene         268.74         266.33         63         2-methyl-1-buttanol         401.85         403.90           10         1.3-butakiene         335.5         378.44         66         2-methyl-1-buttanol         301.40           12         1.3-dichioroporpane         332.55         378.44         66         2-methyl-1-buttanol         373.43         354.43           11         1.4-protophylen glycol         467.55         463.82         7         2-methyl-2-buttanol         372.15         392.53           12	1	1.1-dichloropropane	361.25	370.60	55	2.bromobutane	364.37	364.15
$  \begin{array}{ccccccccccccccccccccccccccccccccccc$	2	1.1-diphenylethane	545.78	534.34	56	Bromopropane	332.56	335.11
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3	1.2.3.4-tetrahydronaphtalene	480.77	460.98	57	2-ethylbutyric acid	466.95	480.82
	4	1.2.3-trimethylbenzene	449.27	429.56	58	2-ethyloutyne aeld	419.65	407.26
	5	1.2.4-trimethylbenzene	442.53	429.76	50 59	2-ethyl-1-butene	337.82	334.28
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	6	1 2-dichloropropene	361.25	386 77	60	2-ethyl-1-beyanol	457.75	473 15
a         1.2-propylene glycol         460.75         471.65         62         2-bexanol         410.10         420.85           9         1.3-butadiene         268.74         263.53         63         2-bexanol         400.85         403.59           1.3-butadiene         268.74         263.53         63         2-bexanol         401.85         413.39           11         1.3-cyclohexadiene         333.49         351.43         65         2-methyl-1-butanol         421.15         430.79           13         1.3-propylene glycol         487.55         463.82         67         2-methyl-1-pentanol         421.15         430.43           14         1.4-butaneciol         501.15         495.92         68         2-methyl-2-pentene         340.45         335.41           15         1.4-dichorobutane         473.15         426.31         70         2-methyl-2-pentene         340.43         332.41         332.17           15         1.4-butaneciol         516.15         515.23         73         2-methylbylentane         333.41         332.47           14         1-choromobutane         374.75         366.81         74         2-methylbylentane         412.44         411.60           21         1-b	7	1 2-diphenylethane	553.65	534.66	61	2-ethyleevyl acrylate	437.73	506.49
b         1.1-b         1.	8	1.2-propylene glycol	460 75	471.65	62	2 hexanol	409.13	423.06
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	9	1.3-butadiene	268 74	263 53	62	2-hexanon	413.04	423.90
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	10	1.3-butanediol	480.15	477.29	64	2-nexanone 2 mathyl 1 hyteral	400.83	405.39
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	10	1.3-cyclohevadiene	353.40	351.43	64	2-methyl-1-butanol	401.83	411.59
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	12	1.3 dichloropropage	303.49	378.04	65	2-methyl-1-butene	304.30	301.40
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	12	1.3 propulane glucol	187 55	163.87	00	2-methyl-1-pentanol	421.15	430.79
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	13	1,3-propyrene grycor	501.15	405.82	0/	2-methyl-1-pentene	335.25	334.43
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	14	1,4-butanedioi	JULIJ 427.05	439.32	68	2-methyl-2-butanol	375.15	395.58
10       1.5-definition of the state state of the state state of the state of the	15	1,4-dichlenenentene	427.03	405.14	69 70	2-methyl-2-pentene	340.45	335.41
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	10	1,5-dichioropentane	455.15	420.31	70	2-methyl-3-ethylpentene	388.80	388.13
18       1,3-pentaneciol       312.15       487.71       72       2-methylpextane       363.20       362.17         10       1,6-bexanediol       516.15       515.23       73       2-methylpentane       332.17         20       1-bromobutane       374.75       366.81       74       2-methylpentane       332.17         21       1-butene       266.90       262.52       76       2-pentanone       375.46       377.82         23       1-chloroputane       381.54       370.42       78       3,3-ditethylpentane       419.34       411.69         24       1-choroputane       381.54       370.42       78       3,3-ditethylpentane       419.34       411.69         25       1-decene       443.75       436.29       80       3-chloropropene       318.11       310.86         27       1-docdecane       486.50       476.66       81       3-hexanone       396.65       394.74         30       1-hexanel       401.45       398.22       84       3-methyl-1-butene       23.21       300.41         30       1-hexanel       401.45       398.22       84       3-methyl-2-butene       311.71       302.56         31       1-hexanel <td< td=""><td>1/</td><td>1,5-nexadiene</td><td>512.15</td><td>334.84</td><td>71</td><td>2-methylbutyric acid</td><td>450.15</td><td>459.79</td></td<>	1/	1,5-nexadiene	512.15	334.84	71	2-methylbutyric acid	450.15	459.79
$\begin{array}{llllllllllllllllllllllllllllllllllll$	18	1,5-pentanedioi	512.15	487.71	72	2-methylhexane	363.20	362.17
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	19	1,6-hexanediol	516.15	515.23	73	2-methylpentane	333.41	332.77
211-bromopropane $341.15$ $33.93$ 752-pentanol $392.15$ $398.85$ 211-butene $266.90$ $262.52$ 762-pentanone $375.46$ $377.82$ 231-chloropentane $351.58$ $341.94$ 772-propanol $355.41$ $344.97$ 241-chloropentane $381.54$ $370.42$ 78 $3.3$ -direthylp-1-butene $419.34$ $411.69$ 251-decene $443.75$ $436.29$ $80$ $3-chloropropene$ $318.11$ $310.86$ 271-doceane $486.50$ $476.66$ $81$ $3$ -hexanone $396.65$ $394.74$ 281-heptene $366.79$ $363.34$ $82$ $3$ -methyl-1-butanol $404.35$ $407.36$ 291-hexadecene $558.02$ $545.13$ $83$ $3$ -methyl-1-butanol $404.35$ $407.36$ 301-hexanal $401.45$ $398.22$ $84$ $3$ -methyl-1-butanol $384.65$ $403.43$ 311-hexanol $430.15$ $429.46$ $85$ $3$ -methyl-2-butanol $384.65$ $403.43$ 311-hexanol $430.15$ $429.46$ $85$ $3$ -methyl-2-butanol $384.65$ $403.43$ 311-hexanol $430.15$ $429.46$ $85$ $3$ -methyl-2-butanol $384.65$ $403.43$ 321-hexanol $430.15$ $429.78$ $88$ $3$ -methyl-2-butanol $384.65$ $403.43$ 331-octane $394.44$ $389.78$ $88$ $3$ -methyl-2-putanol $384.45$ $391.41$ <td>20</td> <td>1-bromobutane</td> <td>3/4./5</td> <td>366.81</td> <td>74</td> <td>2-methylpyridine</td> <td>402.55</td> <td>417.62</td>	20	1-bromobutane	3/4./5	366.81	74	2-methylpyridine	402.55	417.62
221-buttene266.90262.52762-pentanone375.46377.82231-chlorobutane351.58341.94772-propanol355.41344.97241-chloropentane381.54370.42783,3-dittplylpentane419.34411.69251-decanol503.35505.57793,3-dittplylpentane314.40332.77261-decene443.75436.29803-chloropropene318.11310.86271-dodecane486.50476.66813-hexanone396.65394.74281-heptene366.79363.34823-methyl-1-butanol404.35407.36291-hexane366.79363.34823-methyl-1-butane293.21300.41301-hexanol401.45398.22843-methyl-1-butane324.64403.45311-hexanol430.15429.46853-methyl-2-butanol384.65403.43321-hexane336.63334.05863-methyl-bentane336.42332.67331-octadecene587.97574.99873-methyl-bentane336.42332.67341-octene303.11300.95903-pentanol388.45391.41371-tetradecene524.25512.63914-methyl-1-pentene227.01333.63382.2.3.3-tetramethylpentane354.03360.84934-methyl-1-pentene227.01333.63 <tr< td=""><td>21</td><td>l-bromopropane</td><td>344.15</td><td>337.93</td><td>75</td><td>2-pentanol</td><td>392.15</td><td>398.85</td></tr<>	21	l-bromopropane	344.15	337.93	75	2-pentanol	392.15	398.85
231-chlorobutane351.58341.94772-propanol355.4134.49.7241-chloropentane381.54370.42783,3-ditethylpentane419.34411.69251-decanol503.35505.57793,3-ditethylpentane419.34411.69261-decane443.75436.29803-chloropropene318.11310.86271-dodecane486.50476.66813-hexanone396.65394.74281-heptene366.79363.34823-methyl-1-butanol404.35407.36291-hexanal401.45398.22843-methyl-1-pentene227.33333.51311-hexanol430.15429.46853-methyl-2-butanol384.65403.43321-hexene336.63334.05863-methyl-2-butanol384.65302.67331-octadecene587.97574.99873-methyl-pentane336.42332.67341-octene304.11300.95903-pentanol38.45391.41351-pentanol410.95403.55893-methyl-pentane336.42322.67362,2,3-trimethylpentane354.03360.843227.01333.63382,2,3,3-tetramethylpentane413.44410.72924-methyl-pentane327.01336.34392,2,3-trimethylpentane354.03360.843294Acetal376.75407.88<	22	1-butene	266.90	262.52	76	2-pentanone	375.46	377.82
241-chloropentane381.54370.42783.3-dimethylpentane419.34411.69251-decanol503.35505.57793,3-dimethyl-1-butene314.40332.77261-decene443.75436.29803-chloropropene318.11310.86271-dodecane486.50476.66813-hexanone396.65394.74281-heptene366.79363.34823-methyl-1-butanol404.35407.36291-hexadecene558.02545.13833-methyl-1-butene293.21300.41301-hexanal401.45398.22843-methyl-2-butanol384.65403.43311-hexanol430.15429.46853-methyl-2-butene311.71302.56331-octadecene587.97574.99873-methylpentane365.00362.19341-octene394.44389.78883-methylpentane336.42332.67351-pentanol410.95403.55893-methylpentane386.42332.67361-pentene303.11300.95903-pentanol388.45391.41371-tetradecene524.25512.63914-methyl-pentane327.01333.63382,2,3-trimethylpentane354.03360.84934-methylpyrdine418.50418.72402,2,3-trimethylpentane382.09387.5295Acetal376.75407.63 <td>23</td> <td>1-chlorobutane</td> <td>351.58</td> <td>341.94</td> <td>77</td> <td>2-propanol</td> <td>355.41</td> <td>344.97</td>	23	1-chlorobutane	351.58	341.94	77	2-propanol	355.41	344.97
251-decanol503.35505.57793.3-dimethyl-1-butene314.40332.77261-decene443.75436.29803-chloropropene318.11310.86271-dodecane486.50476.66813-hexanone396.65394.74281-heptene366.79363.34823-methyl-1-butanol404.35407.36291-hexanel401.45398.22843-methyl-1-butene293.21300.41301-hexanol430.15429.46843-methyl-2-butanol384.65403.43311-hexanol430.15429.46853-methyl-2-butanol384.65403.43321-hexanol336.63334.05863-methyl-2-butanol384.65403.43321-hexane336.63340.5863-methyl-2-butane311.11302.56331-octane587.97574.99873-methylpentane364.22332.67341-octene394.44389.78883-methylpentane336.42332.17351-pentanol410.95403.55893-methylpentane336.42332.63362,2,3-trimethylpentane413.44410.72924-methyl-1-pentene327.01333.63382,2,3-trimethylpentane354.03367.3694Acetal376.75407.88412,2,4-trimethylpentane382.5393Acetophenone475.15467.632,2,3	24	1-chloropentane	381.54	370.42	78	3,3-diethylpentane	419.34	411.69
261-decene $443.75$ $436.29$ $80$ $3-chlcyanopene$ $318.11$ $310.86$ $27$ 1-dodecane $486.50$ $476.66$ $81$ $3-hexanone$ $996.65$ $394.74$ $28$ 1-heptene $366.07$ $363.34$ $82$ $3-methyl-1-butanol$ $404.35$ $407.36$ $29$ 1-hexanal $401.45$ $398.22$ $84$ $3-methyl-1-butene$ $327.33$ $333.51$ $31$ 1-hexanal $401.45$ $398.22$ $84$ $3-methyl-2-butanel$ $311.71$ $300.41$ $30$ 1-hexanol $401.45$ $398.22$ $84$ $3-methyl-2-butanel$ $311.71$ $302.56$ $31$ 1-hexanol $401.45$ $398.22$ $86$ $3-methyl-2-butanel$ $311.71$ $302.56$ $31$ 1-bexene $336.63$ $334.05$ $86$ $3-methyl-2-butanel$ $311.71$ $302.56$ $31$ 1-octadecene $587.97$ $574.99$ $87$ $3-methyl-2-butanel$ $316.42$ $332.67$ $34$ 1-octadecene $587.97$ $574.99$ $87$ $3-methyl-2-butanel$ $36.42$ $332.67$ $34$ 1-octadecene $587.97$ $574.99$ $87$ $3-methyl-2-butanel$ $316.42$ $332.67$ $35$ 1-pentanol $410.95$ $403.55$ $89$ $3-methylpextanel$ $36.42$ $332.67$ $37$ 1-tetradecene $524.25$ $512.63$ $91$ $4-methyl-2-pentanol$ $408.85$ $491.41$ $37$ $1-tetradecene$ $524.25$ $512.63$ $91$ <t< td=""><td>25</td><td>1-decanol</td><td>503.35</td><td>505.57</td><td>79</td><td>3,3-dimethyl-1-butene</td><td>314.40</td><td>332.77</td></t<>	25	1-decanol	503.35	505.57	79	3,3-dimethyl-1-butene	314.40	332.77
271-dodecane486.50476.66813-hexanone396.65394.74281-heptene366.79363.34823-methyl-1-butanol404.35407.36291-hexadecene558.02545.13833-methyl-1-butanol293.21300.41301-hexanal401.45398.22843-methyl-1-pentene327.33333.51311-hexanol430.15429.46853-methyl-2-butanol384.65403.43321-hexene336.63334.05863-methyl-2-butanol384.65403.43331-octadecene587.97574.99873-methylpexane366.00362.19341-octadecene587.97574.99873-methylpertane336.42332.67351-pentanol410.95403.55893-methylpertane336.42332.67361-pentanol410.95403.55893-methylpyridine417.29417.60361-pentane303.11300.95903-pentanol388.45391.41371-tetradecene524.25512.63914-methyl-1-pentene327.01333.63382,2,3-trimethylpentane354.03360.84934-methyl-2-pentanol404.85422.61392,2,3-trimethylpentane383.00387.3694Acetal376.75407.88412,2,4-trimethylpentane382.0596Acetophenone475.15467.63 <tr< td=""><td>26</td><td>1-decene</td><td>443.75</td><td>436.29</td><td>80</td><td>3-chloropropene</td><td>318.11</td><td>310.86</td></tr<>	26	1-decene	443.75	436.29	80	3-chloropropene	318.11	310.86
281-heptene $366.79$ $363.34$ $82$ $3-methyl-1-butanol$ $404.35$ $407.36$ 291-hexadecene $558.02$ $545.13$ $83$ $3-methyl-1-butene$ $293.21$ $300.41$ 301-hexanal $401.45$ $398.22$ $84$ $3-methyl-1-pentene$ $327.33$ $333.51$ 311-hexanal $430.15$ $429.46$ $85$ $3-methyl-2-butanol$ $384.65$ $403.43$ 321-hexene $336.63$ $334.05$ $86$ $3-methyl-2-butane$ $311.71$ $302.56$ 331-octadecene $887.97$ $574.99$ $87$ $3-methyl-brane$ $365.00$ $362.19$ 341-octene $394.44$ $389.78$ $88$ $3-methyl-prime$ $316.42$ $332.67$ 351-pentanol $410.95$ $403.55$ $89$ $3-methyl-prime$ $372.91$ $333.63$ 361-pentene $303.11$ $300.95$ $90$ $3-pentanol$ $388.45$ $391.41$ 371-tetradecene $524.25$ $512.63$ $91$ $4-methyl-1-pentene$ $327.01$ $333.63$ 38 $2,2,3-trimethyl-pentane$ $354.03$ $360.84$ $93$ $4-methyl-2-pentanol$ $404.85$ $422.61$ 39 $2,2,3-trimethyl-pentane$ $372.39$ $387.52$ $95$ Acctone $329.44$ $320.57$ 42 $2,2-d-imethyl-pentane$ $372.39$ $387.52$ $95$ Acctone $329.44$ $320.57$ 42 $2,2-d-imethyl-pentane$ $386.25$ $406.93$ $96$ Acctoph	27	1-dodecane	486.50	476.66	81	3-hexanone	396.65	394.74
291-hexadecene558.02545.13833-methyl-1-butene293.21300.41301-hexanal401.45398.22843-methyl-1-pentene327.33333.51311-hexanol430.15429.46853-methyl-2-butanol384.65403.43321-hexene336.63334.05863-methyl-2-butene311.71302.56331-octadecene587.97574.99873-methyl-2-butene311.71302.56341-octae394.44389.78883-methyl-pentane36.62332.67351-pentanol410.95403.55893-methyl-pridine417.29417.60361-pentene303.11300.95903-pentanol388.45391.41371-tetradecene524.25512.63914-methyl-1-pentene327.0133.63382,2,3.3.tetramethylpentane413.44410.72924-methyl-2-pentanol404.85422.61392,2,3.trimethylpentane382.00387.3694Acetal376.75407.88412,2,4-trimethylpentane382.28332.0097Acetophenone475.15467.63422,2-dimethyl-1-propanol386.25406.9396Acetophenone475.15467.63432,2-dimethyl-1-putane322.88332.0097Acetylacetone413.55449.81442,3,3-dimethyl-1-butene328.76333.92100Adiponit	28	1-heptene	366.79	363.34	82	3-methyl-1-butanol	404.35	407.36
301-hexanal $401.45$ $398.22$ $84$ $3-methyl-1-pentene$ $327.33$ $333.51$ $31$ 1-hexanol $430.15$ $429.46$ $85$ $3-methyl-2-butanol$ $384.65$ $403.43$ $32$ 1-hexane $336.63$ $334.05$ $86$ $3-methyl-2-butene$ $311.71$ $302.56$ $33$ 1-octadecene $587.97$ $574.99$ $87$ $3-methylpentane$ $365.00$ $362.19$ $34$ 1-octene $394.44$ $389.78$ $88$ $3-methylpentane$ $336.42$ $332.67$ $35$ 1-pentanol $410.95$ $403.55$ $89$ $3-methylpyridine$ $417.29$ $417.60$ $36$ 1-pentene $303.11$ $300.95$ $90$ $3-pentanol$ $388.45$ $391.41$ $37$ 1-tetradecene $524.25$ $512.63$ $91$ $4-methyl-1-pentene$ $327.01$ $333.63$ $32,2,3,3-tetramethylpentane413.44410.72924-methyl-2-pentanol404.85422.61392,2,3-trimethylpentane383.00387.3694Acetal376.75407.88412,2,4-trimethylpentane382.00387.3694Acetal376.75407.88412,2,4-trimethylpentane322.88332.0097Acetophenone475.15467.63422,3-dimethyl-thylentane328.72387.3498Acrylaldehyde325.84340.76452,3-dimethyl-bettene328.76333.92$	29	1-hexadecene	558.02	545.13	83	3-methyl-1-butene	293.21	300.41
311-hexanol430.15429.46853-methyl-2-butanol384.65403.43321-hexene336.63334.05863-methyl-2-butene311.71302.56331-octadecene587.97574.99873-methyl-2-butene366.00362.19341-octane394.44389.78883-methylppentane336.42332.67351-pentanol410.95403.55893-methylpyrdine417.29417.60361-pentene303.11300.95903-pentanol388.45391.41371-tetradecene524.25512.63914-methyl-1-pentene327.01333.63382,2,3,3-tetramethylpentane413.44410.72924-methyl-2-pentanol404.85422.61392,2,3-trimethylbentane384.00387.3694Acetal376.75407.88412,2,4-trimethylpentane372.39387.5295Acetone329.44320.57422,2-dimethyl-1-propanol386.25406.9396Acetophenone475.15467.63432,2-dimethylpentane322.88332.0097Acetophenone413.55449.81442,3,3-dimethylpentane328.7633.92100Adipointrile568.15536.84442,3-dimethyl-1-butene328.7633.92100Adipointrile568.15536.84472,3-dimethyl-2-butene348.75355.3101 $\alpha$ -met	30	1-hexanal	401.45	398.22	84	3-methyl-1-pentene	327.33	333.51
321-hexene $336.63$ $334.05$ $86$ $3-methyl-2-butene$ $311.71$ $302.56$ $33$ 1-octadecene $87.97$ $574.99$ $87$ $3-methylpentane$ $365.00$ $362.19$ $34$ 1-octane $394.44$ $389.78$ $88$ $3-methylpentane$ $336.42$ $332.67$ $35$ 1-pentanol $410.95$ $403.55$ $89$ $3-methylpyridine$ $417.29$ $417.60$ $36$ 1-pentene $303.11$ $300.95$ $90$ $3-pentanol$ $388.45$ $391.41$ $37$ 1-tetradecene $524.25$ $512.63$ $91$ $4-methyl-1-pentene$ $327.01$ $33.63$ $38$ $2,2,3,3$ -tetramethylpentane $413.44$ $410.72$ $92$ $4-methyl-2-pentanol$ $404.85$ $422.61$ $39$ $2,2,3$ -trimethylbutane $354.03$ $360.84$ $93$ $4-methyl-2-pentanol$ $404.85$ $422.61$ $412$ $2,2,3$ -trimethylpentane $383.00$ $387.36$ $94$ Acetal $376.75$ $407.88$ $41$ $2,2,4$ -trimethylpentane $372.39$ $387.52$ $95$ Acetone $329.44$ $320.57$ $42$ $2,2$ -dimethyl-ropanol $386.25$ $406.93$ $96$ Acetophenone $475.15$ $467.63$ $44$ $2,3,3$ -dimethylpentane $322.88$ $332.00$ $97$ Acetyladehyde $325.84$ $340.76$ $45$ $2,3$ -dimethyl-bentene $328.76$ $333.92$ $100$ Adiponitrile $586.15$ $536.84$ $47$ $2,3$ -dimethyl-butene<	31	1-hexanol	430.15	429.46	85	3-methyl-2-butanol	384.65	403.43
331-octadecene $587.97$ $574.99$ $87$ $3$ -methylhexane $365.00$ $362.19$ 341-octene $394.44$ $389.78$ $88$ $3$ -methylpentane $336.42$ $332.67$ 351-pentanol $410.95$ $403.55$ $89$ $3$ -methylpyridine $417.29$ $417.60$ 361-pentene $303.11$ $300.95$ $90$ $3$ -pentanol $388.45$ $391.41$ 371-tetradecene $524.25$ $512.63$ $91$ $4$ -methyl-1-pentene $327.01$ $333.63$ 38 $2,2,3.3$ -tetramethylpentane $413.44$ $410.72$ $92$ $4$ -methyl-2-pentanol $404.85$ $422.61$ 39 $2,2,3$ -trimethylpentane $354.03$ $360.84$ $93$ $4$ -methyl-2-pentanol $404.85$ $422.61$ 40 $2,2,3$ -trimethylpentane $372.39$ $387.36$ $94$ Acetal $376.75$ $407.88$ 41 $2,2,4$ -trimethylpentane $372.39$ $387.52$ $95$ Acetone $329.44$ $320.57$ 42 $2,2$ -dimethyl-1-propanol $386.25$ $406.93$ $96$ Acetophenone $475.15$ $467.63$ 43 $2,2$ -dimethylpentane $387.92$ $387.34$ $98$ Acrylaldehyde $325.84$ $340.76$ 45 $2,3$ -dimethylpentane $387.92$ $387.34$ $98$ Acrylaldehyde $325.84$ $340.76$ 45 $2,3$ -dimethyl-1-butene $328.76$ $333.92$ $100$ Adiponitrile $568.15$ $536.84$ 47 $2,3$ -dimethyl-1-butene $346.35$	32	1-hexene	336.63	334.05	86	3-methyl-2-butene	311.71	302.56
341-octene $394.44$ $389.78$ $88$ $3-methylpentane$ $336.42$ $332.67$ 351-pentanol $410.95$ $403.55$ $89$ $3-methylpyridine$ $417.29$ $417.60$ 361-pentene $303.11$ $300.95$ $90$ $3-pentanol$ $388.45$ $391.41$ 371-tetradecene $524.25$ $512.63$ $91$ $4-methyl-1-pentene$ $327.01$ $333.63$ 38 $2,2,3,3$ -tetramethylpentane $413.44$ $410.72$ $92$ $4-methyl-2-pentanol$ $404.85$ $422.61$ 39 $2,2,3$ -trimethylpentane $383.00$ $387.36$ $94$ Acetal $376.75$ $407.88$ 41 $2,2,3$ -trimethylpentane $383.00$ $387.36$ $94$ Acetal $376.75$ $407.88$ 41 $2,2,4$ -trimethylpentane $382.52$ $95$ Acetone $329.44$ $320.57$ 42 $2,2$ -dimethyl-1-propanol $386.25$ $406.93$ $96$ Acetophenone $475.15$ $467.63$ 43 $2,2$ -dimethylpentane $387.34$ $98$ Acrylacetone $413.55$ $449.81$ 44 $2,3,3$ -dimethylpentane $387.92$ $387.34$ $98$ Acrylacetone $413.55$ $449.81$ 45 $2,3$ -dimethylpentane $328.76$ $333.92$ $100$ Adiponitrile $568.15$ $536.84$ 47 $2,3$ -dimethyl-1-butene $346.35$ $335.78$ $101$ $\alpha$ -methylstyrene $438.65$ $429.56$ 48 $2,3$ -dimethylbutane $331.13$ $332.31$ $103$ A	33	1-octadecene	587.97	574.99	87	3-methylhexane	365.00	362.19
351-pentanol $410.95$ $403.55$ 893-methylpyridine $417.29$ $417.60$ 361-pentene $303.11$ $300.95$ 903-pentanol $388.45$ $391.41$ 371-tetradecene $524.25$ $512.63$ 914-methyl-1-pentene $327.01$ $333.63$ 38 $2,2,3,3$ -tetramethylpentane $413.44$ $410.72$ 924-methyl-2-pentanol $404.85$ $422.61$ 39 $2,2,3$ -trimethylpentane $354.03$ $360.84$ 934-methylpyridine $418.50$ $418.72$ 40 $2,2,3$ -trimethylpentane $383.00$ $387.36$ 94Acetal $376.75$ $407.88$ 41 $2,2,4$ -trimethylpentane $372.39$ $387.52$ 95Acetone $329.44$ $320.57$ 42 $2,2$ -dimethyl-1-propanol $386.25$ $406.93$ 96Acetophenone $475.15$ $467.63$ 43 $2,2$ -dimethylbutane $322.88$ $332.00$ 97Acetylacetone $413.55$ $449.81$ 44 $2,3,3$ -dimethylpentane $387.92$ $387.34$ 98Acrylaldehyde $325.84$ $340.76$ 45 $2,3$ -dimethyl-1-butene $328.76$ $333.92$ 100Adiponitrile $568.15$ $536.84$ 47 $2,3$ -dimethyl-2-butene $346.35$ $335.78$ 101 $\alpha$ -methylstyrene $438.65$ $429.56$ 48 $2,3$ -dimethyl-2-butene $346.35$ $335.78$ 102Allyl alcohol $370.23$ $352.62$ 50 $2,3$ -dimethylbutane $331.13$ $332.31$	34	1-octene	394.44	389.78	88	3-methylpentane	336.42	332.67
$36$ 1-pentene $303.11$ $300.95$ $90$ $3$ -pentanol $388.45$ $391.41$ $37$ 1-tetradecene $524.25$ $512.63$ $91$ $4$ -methyl-1-pentene $327.01$ $333.63$ $38$ $2,2,3,3$ -tetramethylpentane $413.44$ $410.72$ $92$ $4$ -methyl-2-pentanol $404.85$ $422.61$ $39$ $2,2,3$ -trimethylpentane $354.03$ $360.84$ $93$ $4$ -methylpyridine $418.50$ $418.72$ $40$ $2,2,3$ -trimethylpentane $383.00$ $387.36$ $94$ Acetal $376.75$ $407.88$ $41$ $2,2,4$ -trimethylpentane $372.39$ $387.52$ $95$ Acetone $329.44$ $320.57$ $42$ $2,2$ -dimethyl-1-propanol $386.25$ $406.93$ $96$ Acetophenone $475.15$ $467.63$ $43$ $2,2$ -dimethylpentane $322.88$ $332.00$ $97$ Acetylacetone $413.55$ $449.81$ $44$ $2,3,3$ -dimethylpentane $387.92$ $387.34$ $98$ Acrylaldehyde $325.84$ $340.76$ $45$ $2,3$ -butanediol $453.85$ $479.22$ $99$ Acrylaldehyde $325.84$ $340.76$ $47$ $2,3$ -dimethyl-1-butene $328.76$ $333.92$ $100$ Adiponitrile $568.15$ $536.84$ $47$ $2,3$ -dimethyl-2-butene $346.35$ $335.78$ $101$ $\alpha$ -methylstyrene $438.65$ $429.56$ $48$ $2,3$ -dimethylbutane $331.13$ $332.31$ $103$ Allyl alcohol $370.23$ $352.62$ $50$	35	1-pentanol	410.95	403.55	89	3-methylpyridine	417.29	417.60
371-tetradecene $524.25$ $512.63$ $91$ 4-methyl-1-pentene $327.01$ $333.63$ 38 $2,2,3,3$ -tetramethylpentane $413.44$ $410.72$ $92$ 4-methyl-2-pentanol $404.85$ $422.61$ 39 $2,2,3$ -trimethylbutane $354.03$ $360.84$ $93$ 4-methylpyridine $418.50$ $418.72$ 40 $2,2,3$ -trimethylpentane $383.00$ $387.36$ $94$ Acetal $376.75$ $407.88$ 41 $2,2,4$ -trimethylpentane $372.39$ $387.52$ $95$ Acetone $329.44$ $320.57$ 42 $2,2$ -dimethyl-1-propanol $386.25$ $406.93$ $96$ Acetophenone $475.15$ $467.63$ 43 $2,2$ -dimethylbutane $322.88$ $332.00$ $97$ Acetylacetone $413.55$ $449.81$ 44 $2,3,3$ -dimethylpentane $387.92$ $387.34$ $98$ Acrylaldehyde $325.84$ $340.76$ 45 $2,3$ -dimethyl-1-butene $328.76$ $333.92$ $90$ Acrylonitrile $350.50$ $345.85$ 46 $2,3$ -dimethyl-2-butene $346.35$ $335.78$ $101$ $\alpha$ -methylstyrene $438.65$ $429.56$ 48 $2,3$ -dimethyl-3-butadiene-1-ol $341.93$ $335.53$ $102$ Allyl acetate $377.15$ $381.55$ 49 $2,3$ -dimethylbutane $388.76$ $388.22$ $104$ Allyl amine $326.45$ $325.79$ 50 $2,3$ -dimethylbutane $362.93$ $361.66$ $105$ Aniline $457.60$ $435.91$ 51 $2,3$	36	1-pentene	303.11	300.95	90	3-pentanol	388.45	391.41
382,2,3,3-tetramethylpentane413.44410.72924-methyl-2-pentanol404.85422.61392,2,3-trimethylbutane354.03360.84934-methylpyridine418.50418.72402,2,3-trimethylpentane383.00387.3694Acetal376.75407.88412,2,4-trimethylpentane372.39387.5295Acetone329.44320.57422,2-dimethyl-1-propanol386.25406.9396Acetophenone475.15467.63432,2-dimethylbutane322.88332.0097Acetylacetone413.55449.81442,3,3-dimethylpentane387.92387.3498Acrylaldehyde325.84340.76452,3-butanediol453.85479.2299Acrylaldehyde350.50345.85462,3-dimethyl-1-butene328.76333.92100Adiponitrile568.15536.84472,3-dimethyl-2-butene346.35335.78101 $\alpha$ -methylstyrene438.65429.56482,3-dimethyl-abutadiene-1-ol341.93335.53102Allyl acetate377.15381.55492,3-dimethylbutane388.76388.22104Allyl amine326.45325.79512,3dimethylpentane362.93361.66105Aniline457.60435.91522,4,4-trimethyl-1-pentene374.59389.01106Benzaldehyde451.90444.85532,4 4-trimethyl-2	37	1-tetradecene	524.25	512.63	91	4-methyl-1-pentene	327.01	333.63
392,2,3-trimethylbutane354.03360.84934-methylpyridine418.50418.72402,2,3-trimethylpentane383.00387.3694Acetal376.75407.88412,2,4-trimethylpentane372.39387.5295Acetone329.44320.57422,2-dimethyl-1-propanol386.25406.9396Acetophenone475.15467.63432,2-dimethylbutane322.88332.0097Acetylacetone413.55449.81442,3,3-dimethylpentane387.92387.3498Acrylaldehyde325.84340.76452,3-butanediol453.85479.2299Acrylaldehyde350.50345.85462,3-dimethyl-1-butene328.76333.92100Adiponitrile568.15536.84472,3-dimethyl-2-butene346.35335.78101 $\alpha$ -methylstyrene438.65429.56482,3-dimethyl-3-butadiene-1-ol341.93335.53102Allyl acetate377.15381.55492,3-dimethylbutane388.76388.22104Allyl amine326.45325.79512,3dimethylpentane362.93361.66105Aniline457.60435.91522,4,4-trimethyl-1-pentene374.59389.01106Benzaldehyde451.90444.85	38	2,2,3,3-tetramethylpentane	413.44	410.72	92	4-methyl-2-pentanol	404.85	422.61
402,2,3-trimethylpentane383.00 $387.36$ 94Acetal $376.75$ $407.88$ 412,2,4-trimethylpentane $372.39$ $387.52$ 95Acetone $329.44$ $320.57$ 422,2-dimethyl-1-propanol $386.25$ $406.93$ 96Acetophenone $475.15$ $467.63$ 432,2-dimethylbutane $322.88$ $332.00$ 97Acetylacetone $413.55$ $449.81$ 442,3,3-dimethylpentane $387.92$ $387.34$ 98Acrylaldehyde $325.84$ $340.76$ 452,3-butanediol $453.85$ $479.22$ 99Acrylonitrile $350.50$ $345.85$ 462,3-dimethyl-1-butene $328.76$ $333.92$ 100Adiponitrile $568.15$ $536.84$ 472,3-dimethyl-2-butene $346.35$ $335.78$ 101 $\alpha$ -methylstyrene $438.65$ $429.56$ 482,3-dimethylb-3-butadiene-1-ol $341.93$ $335.53$ 102Allyl acetate $377.15$ $381.55$ 492,3-dimethylbexane $388.76$ $388.22$ 104Allyl amine $326.45$ $325.79$ 512,3dimethylpentane $362.93$ $361.66$ 105Aniline $451.90$ $444.85$ 522,4,4-trimethyl-1-pentene $378.06$ $389.52$ $106$ Benzaldehyde $451.90$ $444.85$	39	2,2,3-trimethylbutane	354.03	360.84	93	4-methylpyridine	418.50	418.72
412,2,4-trimethylpentane372.39 $387.52$ 95Acetone $329.44$ $320.57$ 422,2-dimethyl-1-propanol $386.25$ $406.93$ 96Acetophenone $475.15$ $467.63$ 432,2-dimethylbutane $322.88$ $332.00$ 97Acetophenone $413.55$ $449.81$ 442,3,3-dimethylpentane $387.92$ $387.34$ 98Acrylaldehyde $325.84$ $340.76$ 452,3-butanediol $453.85$ $479.22$ 99Acrylaldehyde $325.84$ $340.76$ 462,3-dimethyl-1-butene $328.76$ $333.92$ 100Adiponitrile $568.15$ $536.84$ 472,3-dimethyl-2-butene $346.35$ $335.78$ 101 $\alpha$ -methylstyrene $438.65$ $429.56$ 482,3-dimethyl-3-butadiene-1-ol $341.93$ $335.53$ 102Allyl acetate $377.15$ $381.55$ 492,3-dimethylbutane $331.13$ $332.31$ 103Allyl alcohol $370.23$ $352.62$ 502,3-dimethylhexane $388.76$ $388.22$ 104Allyl amine $326.45$ $325.79$ 512,3dimethylpentane $362.93$ $361.66$ 105Aniline $457.60$ $435.91$ 522,4,4-trimethyl-1-pentene $374.59$ $389.01$ 106Benzaldehyde $451.90$ $444.85$	40	2,2,3-trimethylpentane	383.00	387.36	94	Acetal	376.75	407.88
422,2-dimethyl-1-propanol $386.25$ $406.93$ 96Acetophenone $475.15$ $467.63$ 432,2-dimethylbutane $322.88$ $332.00$ 97Acetophenone $413.55$ $449.81$ 442,3,3-dimethylpentane $387.92$ $387.34$ 98Acrylaldehyde $325.84$ $340.76$ 452,3-butanediol $453.85$ $479.22$ 99Acrylaldehyde $325.84$ $340.76$ 462,3-dimethyl-1-butene $328.76$ $333.92$ 100Adiponitrile $568.15$ $536.84$ 472,3-dimethyl-2-butene $346.35$ $335.78$ 101 $\alpha$ -methylstyrene $438.65$ $429.56$ 482,3-dimethyl-3-butadiene-1-ol $341.93$ $335.53$ 102Allyl acetate $377.15$ $381.55$ 492,3-dimethylbutane $331.13$ $332.31$ 103Allyl alcohol $370.23$ $352.62$ 502,3-dimethylbutane $388.76$ $388.22$ 104Allyl amine $326.45$ $325.79$ 512,3dimethylpentane $362.93$ $361.66$ 105Aniline $457.60$ $435.91$ 522,4,4-trimethyl-1-pentene $374.59$ $389.01$ 106Benzaldehyde $451.90$ $444.85$	41	2,2,4-trimethylpentane	372.39	387.52	95	Acetone	329.44	320.57
432,2-dimethylbutane322.88332.0097Acetylacetone413.55449.81442,3,3-dimethylpentane $387.92$ $387.34$ 98Acrylaldehyde $325.84$ $340.76$ 452,3-butanediol $453.85$ $479.22$ 99Acrylaldehyde $325.84$ $340.76$ 462,3-dimethyl-1-butene $328.76$ $333.92$ 100Adiponitrile $568.15$ $536.84$ 472,3-dimethyl-2-butene $346.35$ $335.78$ 101 $\alpha$ -methylstyrene $438.65$ $429.56$ 482,3-dimethyl-3-butadiene-1-ol $341.93$ $335.53$ 102Allyl acetate $377.15$ $381.55$ 492,3-dimethylbutane $331.13$ $332.31$ 103Allyl alcohol $370.23$ $352.62$ 502,3-dimethylhexane $388.76$ $388.22$ 104Allyl amine $326.45$ $325.79$ 512,3dimethylpentane $362.93$ $361.66$ 105Aniline $451.90$ $444.85$ 53 $2.4$ 4-trimethyl-2-pentene $378.06$ $389.52$ $106$ Benzaldehyde $451.90$ $444.85$	42	2,2-dimethyl-1-propanol	386.25	406.93	96	Acetophenone	475.15	467.63
442,3,3-dimethylpentane387.92387.3498Acrylaldehyde325.84340.76452,3-butanediol453.85479.2299Acrylonitrile350.50345.85462,3-dimethyl-1-butene328.76333.92100Adiponitrile568.15536.84472,3-dimethyl-2-butene346.35335.78101 $\alpha$ -methylstyrene438.65429.56482,3-dimethyl-3-butadiene-1-ol341.93335.53102Allyl acetate377.15381.55492,3-dimethylbutane331.13332.31103Allyl alcohol370.23352.62502,3-dimethylhexane388.76388.22104Allyl amine326.45325.79512,3dimethylpentane362.93361.66105Aniline457.60435.91522,4,4-trimethyl-1-pentene374.59389.01106Benzaldehyde451.90444.85532,44-trimethyl-2-pentene378.06389.52104Alleyle451.90444.85	43	2,2-dimethylbutane	322.88	332.00	97	Acetylacetone	413.55	449.81
452,3-butanediol453.85479.2299Acrylonitrile $350.50$ $345.85$ 462,3-dimethyl-1-butene $328.76$ $333.92$ 100Adiponitrile $568.15$ $536.84$ 472,3-dimethyl-2-butene $346.35$ $335.78$ 101 $\alpha$ -methylstyrene $438.65$ $429.56$ 482,3-dimethyl-3-butadiene-1-ol $341.93$ $335.53$ 102Allyl acetate $377.15$ $381.55$ 492,3-dimethylbutane $331.13$ $332.31$ 103Allyl alcohol $370.23$ $352.62$ 502,3-dimethylhexane $388.76$ $388.22$ 104Allyl amine $326.45$ $325.79$ 512,3dimethylpentane $362.93$ $361.66$ 105Aniline $457.60$ $435.91$ 522,4,4-trimethyl-1-pentene $374.59$ $389.01$ 106Benzaldehyde $451.90$ $444.85$ 532,4 4-trimethyl-2-pentene $378.06$ $389.52$ $106$ Benzaldehyde $451.90$ $444.85$	44	2,3,3-dimethylpentane	387.92	387.34	98	Acrvlaldehvde	325.84	340.76
462,3-dimethyl-1-butene328.76333.92100Adiponitrile568.15536.84472,3-dimethyl-2-butene346.35335.78101 $\alpha$ -methylstyrene438.65429.56482,3-dimethyl-3-butadiene-1-ol341.93335.53102Allyl acetate377.15381.55492,3-dimethylbutane331.13332.31103Allyl alcohol370.23352.62502,3-dimethylhexane388.76388.22104Allyl amine326.45325.79512,3dimethylpentane362.93361.66105Aniline457.60435.91522,4,4-trimethyl-1-pentene374.59389.01106Benzaldehyde451.90444.85532,44-trimethyl-2-pentene378.06389.52104Allyl acetate451.90444.85	45	2,3-butanediol	453.85	479.22	99	Acrylonitrile	350.50	345.85
472,3-dimethyl-2-butene $346.35$ $335.78$ 101 $\alpha$ -methylstyrene $438.65$ $429.56$ 482,3-dimethyl-3-butadiene-1-ol $341.93$ $335.53$ 102Allyl acetate $377.15$ $381.55$ 492,3-dimethylbutane $331.13$ $332.31$ 103Allyl alcohol $370.23$ $352.62$ 502,3-dimethylhexane $388.76$ $388.22$ 104Allyl amine $326.45$ $325.79$ 512,3dimethylpentane $362.93$ $361.66$ 105Aniline $457.60$ $435.91$ 522,4,4-trimethyl-1-pentene $374.59$ $389.01$ 106Benzaldehyde $451.90$ $444.85$ 532,4 4-trimethyl-2-pentene $378.06$ $389.52$ $389.52$ $378.06$ $389.52$ $389.52$ $378.06$ $389.52$	46	2,3-dimethyl-1-butene	328.76	333.92	100	Adiponitrile	568.15	536.84
48       2,3-dimethyl-3-butadiene-1-ol       341.93       335.53       102       Allyl acetate       377.15       381.55         49       2,3-dimethylbutane       331.13       332.31       103       Allyl acetate       370.23       352.62         50       2,3-dimethylbexane       388.76       388.22       104       Allyl amine       326.45       325.79         51       2,3dimethylpentane       362.93       361.66       105       Aniline       457.60       435.91         52       2,4,4-trimethyl-1-pentene       378.06       389.52       106       Benzaldehyde       451.90       444.85	47	2,3-dimethyl-2-butene	346.35	335.78	101	α-methylstyrene	438.65	429.56
49       2,3-dimethylbutane       331.13       332.31       103       Allyl alcohol       370.23       352.62         50       2,3-dimethylbexane       388.76       388.22       104       Allyl amine       326.45       325.79         51       2,3dimethylpentane       362.93       361.66       105       Aniline       457.60       435.91         52       2,4,4-trimethyl-1-pentene       374.59       389.01       106       Benzaldehyde       451.90       444.85         53       2,4 4-trimethyl-2-pentene       378.06       389.52       104       Benzaldehyde       451.90       444.85	48	2.3-dimethyl-3-butadiene-1-ol	341.93	335.53	102	Allyl acetate	377 15	381 55
50       2,3-dimethylhexane       388.76       388.22       104       Allyl amine       326.45       325.79         51       2,3dimethylpentane       362.93       361.66       105       Aniline       457.60       435.91         52       2,4,4-trimethyl-1-pentene       374.59       389.01       106       Benzaldehyde       451.90       444.85         53       2.4.4-trimethyl-2-pentene       378.06       389.52       106       Benzaldehyde       451.90       444.85	49	2.3-dimethylbutane	331.13	332.31	102	Allyl alcohol	370.23	352.62
51       2,3dimethylpentane       362.93       361.66       105       Aniline       457.60       435.91         52       2,4,4-trimethyl-1-pentene       374.59       389.01       106       Benzaldehyde       451.90       444.85         53       2.4 4-trimethyl-2-pentene       378.06       389.52       106       Benzaldehyde       451.90       444.85	50	2.3-dimethylhexane	388.76	388.22	103	Allyl amine	376.25	325 79
52     2,4,4-trimethyl-1-pentene     374.59     389.01     106     Benzaldehyde     451.90     444.85       53     2.4 4-trimethyl-2-pentene     378.06     389.52     106     Benzaldehyde     451.90     444.85	51	2.3dimethylpentane	362.93	361.66	105	Aniline	457 60	435 Q1
53 2.4 4-trimethyl-2-nentene 378.06 389.52	52	2.4.4-trimethyl-1-pentene	374.59	389.01	105	Benzaldebyde	451 00	444 85
	53	2.4.4-trimethyl-2-pentene	378.06	389 52	100	Denzardenyde	TJ1.70	U.U.

Table 3 (continued)

# Table 3 (continued)

Table	3 (	continued)	
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No 107 108 109 110 111 112 113	Compound Benzene Benzoic acid Benzul acetate	<i>T</i> <sub>exp</sub> , K 353.24	<i>T</i> <sub>calc</sub> , K	No	Compound Ethylenecarboxylic acid	<i>T</i> <sub>exp</sub> , K	T <sub>calc</sub> , K
107 108 109 110 111 112 113	Benzene Benzoic acid Benzul acetate	353.24	353.02	161	Ethylenecarboxylic acid	414 15	
108 109 110 111 112 113	Benzoic acid Benzyl acetate		555.02	101	Emplementation yne acid	414.13	426.41
109 110 111 112 113	Benzyl acetate	522.40	519.90	162	Hexamethylene imine	404.85	404.81
110 111 112 113	Denzyr acetaic	486.65	482.88	163	Hexanenitrile	436.75	399.81
111 112 113	Benzyl alcohol	477.85	474.70	164	Isopentane	300.99	299.50
112 113	Benzyl benzoate	596.65	574.98	165	Isobutane	261.43	260.95
113	Bicyclohexyl	512.19	494.28	166	Isobutanol	380.81	381.27
115	Bromobenzene	429.24	435.64	167	Isobutene	266.25	263.26
114	Butyl vinyl ether	366.97	374.40	168	Isobutyl acetate	389.80	405.39
115	Chlorobenzene	404.87	415.27	169	Isobutyl acrylate	405.15	428.66
116	Cis-1,2-dimethylcyclohexane	402.94	401.10	170	Isobutyl formate	371.22	379.94
117	Cis-1,3-dimethylcyclohexane	393.24	401.18	171	Isobutyl	420.65	449.30
118	Cis-1,4-dimethylcylohexane	397.47	401.18	172	Isobutylamine	340.88	353.39
119	Cis-2-butene	276.87	263.97	173	Isobutylbenzene	445.94	449.77
120	Cis-2-hexene	342.03	334.95	174	Isobutyraldehyde	337.25	347.14
121	Cumene	425.56	428.39	175	Isobutyric acid	427.85	441.39
122	Cyclohexane	353.87	348.51	176	Isobutyronitrile	376.76	348.42
123	Cyclohexanol	434.00	444.01	177	Isophorone	488.35	488.74
124	Cyclohexanone	428.90	420.86	178	Isoprene	307.21	302.23
125	Cyclohexylamine	407.65	419.17	179	Isopropyl acetate	361.65	380.90
126	Cyclopentadiene	314.65	317.27	180	Isopropyl chloride	308.85	307.88
127	Cyclopentane	322.40	316.50	181	Isopropyl amine	305.55	315.01
128	Cyclopentene	317.38	316.99	182	Isovaliric acid	448.25	460.20
129	Cyclohexene	356.12	350.12	183	<i>m</i> -cresol	475.43	478.54
130	Di- <i>n</i> -butyl ether	413.44	421.69	184	<i>m</i> -diethylbenzene	454.29	450.45
131	Di- <i>n</i> -hexyl ether	498.85	501.15	185	<i>m</i> -diethylbenzene	476.33	488.61
132	Di- <i>n</i> -propyl ether	362.79	372.57	186	<i>m</i> -ethyltoluene	434.48	429.21
133	Di- <i>n</i> -propylamine	382.00	398.24	187	<i>m</i> -toluidine	476.55	456.36
134	Dibutyl phthalate	613.15	628.67	188	<i>m</i> -xylene	412.27	406.42
135	Dibutyl sebacate	622.15	644.70	189	Mesityl oxide	402.95	402.99
136	Diethyl ether	308.58	312.63	190	Mesitylene	437.89	429.82
137	Diethyl ketone	375.14	371.05	191	Methacrolein	341.15	356.49
138	Diethyl phthalate	567.15	575.18	192	Methyl acrylate	353.35	354.06
139	Diethylamine	328.60	345.50	193	Methyl ethyl ketone	352.79	352.04
140	Diisopropyl ether	341.45	371.83	194	Methyl acetate	330.09	323.20
141	Diisopropylamine	357.05	395.52	195	Methyl ethyl ether	280.05	276.51
142	Dimethylphthalate	556.85	545.55	196	Methyl isobutyl ketone	389.65	396.98
143	Dimethyl terephthalate	561.15	545.78	197	Methyl isobutyl ether	331.70	344.10
144	Diphenyl ether	531.46	525.41	198	Methyl isopropenyl ketone	371.15	383.16
145	Diphenyl amine	575.15	553.96	199	Methyl isopropyl ether	323.75	312.44
146	Diphenylmethane	537.42	518.36	200	Methyl isopropyl ketone	367.55	378.17
147	Divinyl ether	301.45	315.93	201	Methyl <i>n</i> -butyrate	375.90	380.93
148	Ethyl acetate	350.21	353.47	202	Methyl propionate	352.60	353.59
149	Ethyl acrylate	372.65	381.17	203	Methyl <i>sec</i> -butyl ether	332.15	344.08
150	Ethyl benzoate	486.55	482.85	204	Methyl <i>tert</i> -butyl ether	328.35	343.60
151	Ethyl formate	327.46	322.59	205	Methyl <i>tert</i> -pentyl ether	359.45	371.83
152	Ethyl isobutyrate	383.00	405.24	206	Methyl vinyl ether	278.65	279.19
153	Ethyl isopropyl ketone	386.55	398.14	207	Methanal	253.65	228.95
154	Ethyl- <i>n</i> -butyrate	394.65	405.66	208	Methylcyclohexane	374.08	376.11
155	Ethyl propionate	372.25	380.75	209	Methylcyclopentadiene	345.93	348.31
156	Ethyl propyl ether	337.01	344.32	210	Methylcyclopentane	344.96	347.47
157	Ethyl vinyl ether	308.70	314.95	211	N,N-dimethylaniline	466.69	463.90
158	Ethylbenzene	409.35	405.81	212	<i>n</i> -butane	272.65	261.45
159	Ethylcyclohexane	404.95	401.46	213	Butanol	390.81	382.02
160	Ethylcyclopentane	376.62	375.34	214	<i>n</i> -butyl acetate	399.15	405.72

Table 3 (continued)

Table 3	(continued)
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215 $n$ -butyl etryl aterylate       421.00       428.97       269       Propionic acid         216 $n$ -butyl ether       363.35       372.56       270       Propionic acid         217 $n$ -butyl formate       379.25       380.29       271       Propionic acid         218 $n$ -butyl stearate       623.15       660.38       272       Pyridine         219 $n$ -butyl benzene       456.46       450.08       274       Sce-butyl acetate         221 $n$ -butyl benzene       456.46       430.01       275       Sce-butyl acetate         223 $n$ -butyric acid       436.42       439.01       278       Sce-butyl acetate         224 $n$ -butyrointrile       390.75       346.41       278       Sce-butyl anine         224 $n$ -butyrointrile       390.75       346.41       278       Sce-butyl acetate         225 $n$ -docane       449.47       476.21       280       Styrene         227 $n$ -hexane       341.88       332.5       283       Tert-butyl acetate         230 $n$ -hexane       341.88       435.47       751       284       Tert-butyl acetate         231 $n$ -hexane	No	Compound	$T_{\rm exp}$ , K	$T_{\text{calc}}, \mathbf{K}$	No	Compound	
216 $n$ -butyl ether       365.35       372.56       270       Propionitrile         217 $n$ -butyl formate       379.25       380.29       271       Propylene         218 $n$ -butyl stearate       632.15       660.38       274       Sec-butyl accetate         220 $n$ -butylexpcohexane       456.46       450.08       274       Sec-butyl accetate         221 $n$ -butylexpcohexane       454.13       446.21       275       Sec-butyl accetate         223 $n$ -butyraidelyde       347.95       348.42       276       Sec-butyl banzene         224 $n$ -butyronitrile       390.75       346.41       278       Sec-butyl benzene         225 $n$ -decane       447.30       435.76       279       Stearic acid         226 $n$ -docane       489.47       476.21       280       Styrene         227 $n$ -hexano       341.88       333.25       283       Terr-butyl acctate         230 $n$ -hexano       341.88       333.25       284       Ter-butyl acctate         231 $n$ -nonane       423.97       413.36       284       Terr-butyl acctate         233 $n$ -nonane       398.83	215	<i>n</i> -butyl acrylate	421.00	428.97	269	Propionic acid	
217 <i>n</i> -butyl stearate       370.25       380.29       271       Propylene         218 <i>n</i> -butyl stearate       623.15       660.38       272       Pyridine         219 <i>n</i> -butyl parine       350.55       352.03       273       Quinoline         220 <i>n</i> -butyl parine       456.46       450.08       274       Sec-butyl alcohol         221 <i>n</i> -butyrialchyde       347.95       348.42       275       Sec-butyl chloride         221 <i>n</i> -butyrialchyde       347.95       346.41       278       Sec-butyl chloride         223 <i>n</i> -butyrointrile       390.75       346.41       278       Sec-butyl actate         226 <i>n</i> -deceane       487.30       435.76       281       Terr-butyl actate         226 <i>n</i> -bexadecane       560.01       544.79       282       Terr-butyl actate         230 <i>n</i> -hexanoic acid       478.88       475.51       284       Terr-butyl chloride         231 <i>n</i> -nonac       423.97       413.36       287       Trah-butyl barnene         232 <i>n</i> -nonac       423.97       413.36       287       Trans-1,2-dimethyl         233 <i>n</i> -ortalcecane       589.8	216	<i>n</i> -butyl ethyl ether	365.35	372.56	270	Propionitrile	
218 $n$ -butyl stearate       623.15       660.38       272       Pyridine         219 $n$ -butylamine       350.55       352.03       273       Quinoline         219 $n$ -butylexplohexane       454.13       446.21       275       Sec-butyl acetate         221 $n$ -butyraldehyde       347.95       348.42       276       Sec-butyl ancetate         221 $n$ -butyraldehyde       347.95       346.41       278       Sec-butyl ancetate         223 $n$ -doctane       449.73       346.41       278       Sec-butyl ancetate         225 $n$ -doctane       449.73       346.41       278       Sec-butyl ancetate         226 $n$ -doctane       349.47       280       Styrene       281       Tert-butyl acetate         228 $n$ -hexadecane       560.01       544.79       282       Tert-butyl acetate       281       287       Tert-butyl acetate         230 $n$ -hexanoic acid       478.85       475.51       284       Tert-butyl alchoide         231 $n$ -hexane       630.05       588.78       286       Tert-butyl achide         231 $n$ -nonadecane       589.86       574.68       288       Trans-1,2	217	<i>n</i> -butyl formate	379.25	380.29	271	Propylene	
219 $n$ -butylamine       350.55       352.03       273       Quinoline         220 $n$ -butylbenzene       456.46       450.08       274       Sec-butyl acotate         210 $n$ -butyraldehyde       347.95       348.42       276       Sec-butyl alcohol         221 $n$ -butyronitrile       390.75       346.41       278       Sec-butyl chloride         223 $n$ -butyronitrile       390.75       346.41       278       Sec-butyl chloride         224 $n$ -dudecane       449.47       476.21       280       Styrene         225 $n$ -decane       449.47       476.21       280       Styrene         226 $n$ -hexanoic acid       478.85       281       Terr-butyl alcohol         229 $n$ -hexanoic acid       478.85       447.51       284       Terr-butyl alcohol         230 $n$ -nonadecane       603.05       588.78       286       Terns-1,2-dimethyl         231 $n$ -notadecane       599.86       574.68       287       Tolucne         234 $n$ -octane       398.83       389.13       289       Trans-1,2-dimethyl         235 $n$ -pentae       309.23       300.04       290<	218	<i>n</i> -butyl stearate	623.15	660.38	272	Pyridine	
220 $n$ -butylbenzene       456.46       450.08       274       Sec-butyl alcothol         221 $n$ -butyrclohexane       454.13       446.21       275       Sec-butyl alcothol         221 $n$ -butyrclohexane       454.13       446.21       275       Sec-butyl chloride         223 $n$ -butyrclohexane       437.95       348.42       276       Sec-butyl chloride         224 $n$ -butyrcloit       390.75       346.41       278       Sec-butyl chloride         225 $n$ -deceane       447.30       435.76       279       Stearic acid         226 $n$ -deceane       390.75       346.41       278       Sec-butyl chloride         226 $n$ -deceane       489.47       476.21       280       Styrene         227 $n$ -hexane       331.25       283       Tert-butyl chloride         230 $n$ -hexane       341.88       333.25       284       Tert-butyl chloride         231 $n$ -nonadecane       603.05       588.78       286       Tert-butyl chloride         231 $n$ -nonadecane       389.83       391.3       287       Trans-1,2-dimethyl         233 $n$ -nonane       389.83       380.12<	219	<i>n</i> -butylamine	350.55	352.03	273	Quinoline	
221 $n$ -buty(c)c)chocane       454,13       446,21       275       Sec-buty1 alcohol         222 $n$ -butyraidehyde       347,95       348,42       276       Sec-buty1 chloride         223 $n$ -butyrointrile       390,75       346,41       277       Sec-buty1 benzene         225 $n$ -decane       447,30       435,76       279       Stearic acid         226 $n$ -docdecane       449,47       476,21       280       Styrene         227 $n$ -hexane       361,83       332,52       283       Terr-buty1 acotate         228 $n$ -hexane       341,88       333,25       283       Terr-buty1 acotate         229 $n$ -hexane       436,45       404,74       285       Terr-buty1 chloride         231 $n$ -nonane       423,97       413,36       287       Toluene         234 $n$ -octadecane       589,86       574,68       288       Trans-1,4-dimethy1         235 $n$ -octate       399,83       389,13       289       Trans-2-butene         235 $n$ -octate       398,23       380,04       290       Trans-2-butene         236 $n$ -penty1 formate       306,04       293	220	<i>n</i> -butylbenzene	456.46	450.08	274	Sec-butyl acetate	
222 $n$ -butyraldehyde       347.95       348.42       276       Sec-butyl choirde         223 $n$ -butyronitrile       390.75       346.41       278       Sec-butyl benzene         224 $n$ -butyronitrile       390.75       346.41       278       Sec-butyl benzene         225 $n$ -decane       447.30       435.76       279       Stearic acid         226 $n$ -docdecane       489.47       476.21       280       Styrene         227 $n$ -hexalecane       560.01       544.79       282       Terr-butyl acetate         228 $n$ -hexanoic acid       478.85       475.51       284       Terr-butyl choride         230 $n$ -hexylamine       404.65       404.74       285       Terr-butyl choride         231 $n$ -nonadecane       603.05       588.78       286       Tetrahydrofuran         233 $n$ -octadecane       589.86       574.68       287       Toluene         234 $n$ -octadecane       398.83       389.13       289       Trans-1,2-dimethyl         236 $n$ -pental       309.23       300.04       290       Trans-2-hexene         238 $n$ -pentyl formate       370.35	221	<i>n</i> -butylcyclohexane	454.13	446.21	275	Sec-butyl alcoho	1
223 $n$ -butyre acid       436.42       439.01       277       Sec-butyl annine         224 $n$ -butyronitrile       390.75       346.41       278       Sec-butyl benzene         225 $n$ -decane       447.30       435.76       279       Stearic acid         226 $n$ -dodecane       489.47       476.21       280       Styrene         227 $n$ -hexane       341.88       332.25       283       Terr-butyl acholol         229 $n$ -hexanoic acid       478.85       475.51       284       Terr-butyl chloride         231 $n$ -nonadecane       603.05       588.78       286       Tertarbutyl chloride         231 $n$ -nonadecane       398.83       399.13       287       Toluene         234 $n$ -octade       398.83       380.12       292       Trans-1,4-dimethyl         235 $n$ -octane       398.83       380.12       292       Trans-2-butene         238 $n$ -pentyl formate       374.65       380.81       295       Valeronitrile         236 $n$ -pentyl formate       374.65       380.81       295       Valeronitrile         239       Propanol       370.35       352.65	222	<i>n</i> -butyraldehyde	347.95	348.42	276	Sec-butyl chlorid	e
224 $n$ -butyronitrile       390.75       346.41       278       Sec-butyl benzene         225 $n$ -decane       447.30       435.76       279       Stearic acid         226 $n$ -docdecane       489.47       476.21       280       Styrene         227 $n$ -hexane       311.88       362.63       281       Terr-butyl acotate         228 $n$ -hexanoic acid       478.85       475.51       284       Terr-butyl acotate         230 $n$ -hexanoic acid       478.85       475.51       284       Terr-butyl acotate         231 $n$ -nonadecane       603.05       588.78       286       Tertastryl acotate         233 $n$ -nonane       423.97       413.36       287       Toluene         234 $n$ -octate       398.83       389.13       289       Trans-1,2-dimethyl         235 $n$ -pentane       309.23       300.04       290       Trans-2-butene         238 $n$ -pentyl formate       406.60       405.24       291       Trans-2-butene         236 $n$ -pentyl formate       371.65       380.12       292       Trans-2-butene         239       Prasoprojonaldehyde       321.15       31	223	<i>n</i> -butyric acid	436.42	439.01	277	Sec-butyl amine	
225 $n$ -decane       447.30       435.76       279       Stearic acid         226 $n$ -dodecane       489.47       476.21       280       Styrene         227 $n$ -hextance       360.63       281       Terr-butyl acetate         228 $n$ -hexanoic acid       478.85       475.51       283       Terr-butyl chloride         230 $n$ -hexanoic acid       478.85       475.51       284       Terr-butyl chloride         231 $n$ -hexylamine       404.65       404.74       285       Terr-butyl benzene         231 $n$ -hexylamine       423.97       413.36       287       Toluene         233 $n$ -notadecane       598.86       574.68       288       Trans-1.2-dimethyl         235 $n$ -octane       398.83       389.13       289       Trans-1.4-dimethyl         236 $n$ -pentyl formate       406.60       405.24       291       Trans-2-bacene         238 $n$ -pentyl formate       370.35       352.65       293       Trans-2-bacene         237 $n$ -propyl acteate       374.65       380.12       295       Valeralethyla         241 $n$ -propyl formate       353.97       353.13	224	<i>n</i> -butyronitrile	390.75	346.41	278	Sec-butyl benzen	e
226 $n$ -heptane       371.58       362.63       281       Tert-butyl acetate         227 $n$ -hexance       560.01       544.79       282       Tert-butyl acetate         228 $n$ -hexance       341.88       333.25       283       Tert-butyl acetate         230 $n$ -hexance       404.65       404.74       285       Tert-butyl chloride         231 $n$ -hexance       603.05       588.78       286       Tert-butylenzene         231 $n$ -nonadecane       603.05       588.78       286       Tert-butylenzene         234 $n$ -oncatace       398.86       574.68       288       Trans-1,2-dimethyl         235 $n$ -octatae       398.93       389.13       289       Trans-1,2-dimethyl         236 $n$ -pentae       309.23       300.04       290       Trans-2-butene         238 $n$ -pentyl formate       406.60       405.24       291       Trans-2-butene         237 $n$ -pentyl formate       370.35       352.65       293       Trans-2-butene         239       Propanol       370.35       352.65       293       Trans-2-butene         240 $n$ -propyl choloride       319.67 <t< td=""><td>225</td><td><i>n</i>-decane</td><td>447.30</td><td>435.76</td><td>279</td><td>Stearic acid</td><td></td></t<>	225	<i>n</i> -decane	447.30	435.76	279	Stearic acid	
227 $n$ -heptane       371.58       362.63       281 $Tert$ -butyl acetate         228 $n$ -hexane       361.85       333.25       283 $Tert$ -butyl chloride         230 $n$ -hexanoic acid       478.85       475.51       284 $Tert$ -butyl chloride         231 $n$ -nonadecane       603.05       588.78       286 $Tert$ -butyl ofteran         233 $n$ -nonane       423.97       413.36       287 $Toluene$ 234 $n$ -octatecane       589.86       574.68       288 $Trans-1,2$ -dimethyl         236 $n$ -pentane       398.83       389.13       289 $Trans-1,3$ -dimethyl         237 $n$ -pentane       390.23       300.04       290 $Trans-1,4$ -dimethyl         237 $n$ -pentyl formate       406.60       405.24       291 $Trans-2$ -butene         238 $n$ -pentyl formate       370.35       352.65       293 $Trans-2$ -butene         239       Propanol       370.35       353.13       297       Valeronitrile         241 $n$ -propyl chloride       319.67       309.94       296       Valeronitrile         244 $n$ -propyl propionate	226	<i>n</i> -dodecane	489.47	476.21	280	Styrene	
228 $n$ -hexadecane       560.01       544.79       282       Tert-buty alcohol         229 $n$ -hexanoic acid       478.85       475.51       283       Tert-butyl chioride         230 $n$ -hexanoic acid       478.85       475.51       284       Tert-butyl emine         231 $n$ -hexylamine       404.65       404.74       285       Tert-butylenzene         232 $n$ -nonadecane       603.05       588.78       286       Tetrahydrofuran         233 $n$ -octane       398.83       389.13       289       Trans-1,2-dimethyl         234 $n$ -octane       398.83       380.13       289       Trans-1,3-dimethyl         235 $n$ -octane       398.83       380.12       290       Trans-2-butene         238 $n$ -pentyl formate       406.60       405.24       291       Trans-2-butene         236 $n$ -pentyl formate       370.35       352.65       293       Trans-2-bexene         239       Propanol       370.35       352.165       293       Trans-2-bexene         240 $n$ -propyl acctate       374.65       380.81       295       Valeraldehyde         241 $n$ -propyl propionate       395.6	227	<i>n</i> -heptane	371.58	362.63	281	Tert-butyl acetate	•
229 $n$ -hexane       341.88       333.25       283       Tert-butyl chloride         230 $n$ -hexanoic acid       478.85       475.51       284       Tert-butyl amine         231 $n$ -hexanoic acid       478.85       475.51       284       Tert-butyl enloride         231 $n$ -nexalaccane       603.05       588.78       286       Tetrahydrofuran         233 $n$ -nonadecane       589.86       574.68       288       Trans-1,2-dimethyl         234 $n$ -octatee       398.83       389.13       289       Trans-1,2-dimethyl         235 $n$ -octate       309.23       300.04       290       Trans-1,2-dimethyl         236 $n$ -pentyl formate       406.60       405.24       291       Trans-2-butene         239       Propanol       370.35       352.65       293       Trans-crotonic aci         240 $n$ -propyl acetate       374.65       380.81       295       Valeraidehyde         241 $n$ -propyl formate       353.97       353.13       297       Valeronitrile         244 $n$ -propyl propionate       392.65       405.66       298       Vinyl acetate         244 $n$ -propyl propionate	228	<i>n</i> -hexadecane	560.01	544.79	282	Tert-buty alcohol	l
230 $n$ -hexanoic acid       478.85       475.51       284       Tert-butyl amine         231 $n$ -hoxalaceane       603.05       588.78       286       Tetrahydrofuran         233 $n$ -nonane       423.97       413.36       287       Toluene         234 $n$ -octadecane       589.86       574.68       288       Trans-1,2-dimethyl         236 $n$ -octadecane       398.83       389.13       289       Trans-1,2-dimethyl         236 $n$ -pentyl formate       406.60       405.24       291       Trans-1,4-dimethyl         237 $n$ -pentyl formate       309.23       300.04       290       Trans-1,4-dimethyl         238 $n$ -pentyl formate       370.55       380.81       292       Trans-2-batene         239       Propanol       370.35       352.65       293       Trans-crotonoic aci         240 $n$ -propyl actate       374.65       380.81       295       Valeraldehyde         241 $n$ -propyl propionate       395.65       405.66       298       Vinyl acetate         243 $n$ -propyl propionate       395.65       320.40       No       Compound       Tert-buylylylylylylylylylylylylylylylylylylyl	229	<i>n</i> -hexane	341.88	333.25	283	Tert-butyl chlorid	le
231 $n$ -hexylamine       404.65       404.74       285       Tert-butylbenzene         232 $n$ -nonadecane       603.05       588.78       286       Tetrahydtrofuran         233 $n$ -nonane       423.97       413.36       287       Toluene         234 $n$ -octadecane       589.86       574.68       288       Trans-1,2-dimethyl         235 $n$ -octane       399.83       389.13       289       Trans-1,3-dimethyl         236 $n$ -pentane       309.23       300.04       290       Trans-1,4-dimethyl         237 $n$ -pentyl formate       406.60       405.24       291       Trans-2-butene         238 $n$ -pentyl formate       370.55       380.12       292       Trans-2-butene         239       Propanol       370.35       352.65       293       Trans-cotonoic aci         241 $n$ -propyl cetate       374.65       380.81       295       Valeraldehyde         242 $n$ -propyl formate       353.97       353.13       297       Valeronitrile         244 $n$ -propyl propionate       395.65       405.66       298       Vinyl acetate         247 $n$ -propyl propionate       422.39 <td>230</td> <td>n-hexanoic acid</td> <td>478.85</td> <td>475.51</td> <td>284</td> <td>Tert-butyl amine</td> <td></td>	230	n-hexanoic acid	478.85	475.51	284	Tert-butyl amine	
232 $n$ -nonane       603.05       588.78       286       Tetrahydrofuran         233 $n$ -nonane       423.97       413.36       287       Tolucne         234 $n$ -octaae       589.86       574.68       288       Trans-1,2-dimethyl         235 $n$ -octane       309.23       300.04       290       Trans-1,3-dimethyl         237 $n$ -pentane       309.23       300.04       290       Trans-1,4-dimethyl         238 $n$ -pentyl formate       406.60       405.24       291       Trans-2-butene         239       Propanol       370.35       352.65       293       Trans-2-bexene         240 $n$ -propyl acetate       374.65       380.81       295       Valeraldehyde         241 $n$ -propyl formate       395.65       405.66       298       Vinyl acetate         244 $n$ -propyl propionate       395.65       405.66       298       Vinyl acetate         245 $n$ -propyl propionate       321.65       312.20       Table 4       Experimental vs         246 $n$ -propylexclohexane       429.90       424.59       inorganics using Eq. (9) wi       No         248 $n$ -propylexclohexane <t< td=""><td>231</td><td><i>n</i>-hexylamine</td><td>404.65</td><td>404.74</td><td>285</td><td>Tert-butylbenzen</td><td>e</td></t<>	231	<i>n</i> -hexylamine	404.65	404.74	285	Tert-butylbenzen	e
233       n-nonane       423.97       413.36       287       Toluene         234       n-octadecane       589.86       574.68       288       Trans-1,2-dimethyl         235       n-octane       398.83       389.13       289       Trans-1,3-dimethyl         236       n-pentyl       formate       406.60       405.24       291       Trans-1,4-dimethyl         237       n-pentylamine       377.65       380.12       292       Trans-2-butene         238       n-pentylamine       377.65       380.12       292       Trans-2-hexene         239       Propanol       370.35       352.65       293       Trans-crotonoic aci         240       n-propil acetate       374.65       380.81       295       Valeric acid         241       n-propyl endicide       319.67       309.94       296       Valeric acid         243       n-propyl propionate       395.65       405.66       298       Vinyl acetate         244       n-propyl propionate       321.65       322.04       Trake 4       Experimental vs         244       n-propylexclopentane       422.39       428.72       Table 4       Experimental vs         250       Neopentane       282.65	232	<i>n</i> -nonadecane	603.05	588.78	286	Tetrahydrofuran	
234       n-octadecane       589.86       574.68       288       Trans-1,2-dimethyl         235       n-octane       398.83       389.13       289       Trans-1,3-dimethyl         236       n-pentyl formate       406.60       405.24       291       Trans-2-butene         237       n-pentyl formate       406.60       405.24       291       Trans-2-butene         238       n-pentyl formate       377.65       380.12       292       Trans-2-butene         239       Propanol       370.35       352.65       293       Trans-crotonoic aci         240       n-propinaldehyde       321.15       317.36       294       Trimethylamine         241       n-propyl acetate       374.65       380.81       295       Valeric acid         243       n-propyl propionate       395.65       405.66       298       Vinyl acetate         243       n-propyl propionate       321.65       322.04       Trans-izene       1         244       n-propylexclopentane       428.79       428.72       Table 4       Experimental vs         244       n-propylexclopentane       428.65       298.79       1       H_2O       37         250       Neopentyl glycol       <	233	<i>n</i> -nonane	423.97	413.36	287	Toluene	
235 <i>n</i> -octane398.83389.13289 <i>Trans</i> -1,3-dimethyl236 <i>n</i> -pentane309.23300.04290 <i>Trans</i> -1,4-dimethyl237 <i>n</i> -pentyl formate406.60405.24291 <i>Trans</i> -2-butene238 <i>n</i> -pentylamine377.65380.12292 <i>Trans</i> -2-hexene239Propanol370.35352.65293 <i>Trans</i> -crotonoic aci240 <i>n</i> -propionaldehyde321.15317.36294Trimethylamine241 <i>n</i> -propyl acetate374.65380.81295Valeraldehyde242 <i>n</i> -propyl propionate395.65405.66298Valerointrile244 <i>n</i> -propyl propionate392.65322.04296Valerointrile245 <i>n</i> -propyl propionate422.90424.59inorganics using Eq. (9) wi246 <i>n</i> -propyl cyclopentane404.11400.72MoCompound <i>Te</i> 247 <i>n</i> -propyl glycol483.00496.792H <sub>2</sub> O <sub>2</sub> 42250Neopentane282.65298.791H <sub>2</sub> O37251Neopentyl glycol483.00496.792H <sub>2</sub> O <sub>2</sub> 42253 <i>o</i> -dichlorobenzene455.57465.943NH <sub>3</sub> 24254 <i>o</i> -dichlybenzene456.61450.275NH <sub>2</sub> OH38255 <i>o</i> -ethyltoluene473.55449.396HCN29257 <i>o</i> -stylene417.58406.397CH <sub>3</sub> F1925	234	<i>n</i> -octadecane	589.86	574.68	288	Trans-1,2-dimeth	ylcycloh
236 <i>n</i> -pentane       309.23       300.04       290 <i>Trans</i> -1,4-dimethyl         237 <i>n</i> -pentyl formate       406.60       405.24       291 <i>Trans</i> -2-butene         238 <i>n</i> -pentylamine       377.65       380.12       292 <i>Trans</i> -2-bexene         239       Propanol       370.35       352.65       293 <i>Trans</i> -2-bexene         240 <i>n</i> -propyl actate       374.65       380.81       295       Valeraldehyde         241 <i>n</i> -propyl chloride       319.67       309.94       296       Valeraidehyde         242 <i>n</i> -propyl chloride       319.67       309.94       296       Valeraidehyde         243 <i>n</i> -propyl propionate       395.65       405.66       298       Vinyl acetate         244 <i>n</i> -propyl propionate       321.65       322.04       Table 4       Experimental vs         246 <i>n</i> -propyllexpene       404.11       400.72       Table 4       Experimental vs         247 <i>n</i> -propylexpentane       404.11       400.72       Table 4       Experimental vs         250       Neopentane       282.65       298.79       Table 4       Experimental vs         251       Neopenty	235	<i>n</i> -octane	398.83	389.13	289	Trans-1,3-dimeth	ylcycloh
237 <i>n</i> -pentyl formate       406.60       405.24       291 <i>Trans-2</i> -butene         238 <i>n</i> -pentylamine       377.65       380.12       292 <i>Trans-2</i> -hexene         239       Propanol       370.35       352.65       293 <i>Trans-2</i> -hexene         240 <i>n</i> -propioladehyde       321.15       317.36       294       Trimethylamine         241 <i>n</i> -propyl acetate       374.65       380.81       295       Valeraldehyde         242 <i>n</i> -propyl acetate       353.97       353.13       297       Valeronitrile         243 <i>n</i> -propyl propionate       395.65       405.66       298       Vinyl acetate         244 <i>n</i> -propylenzene       432.39       428.72       Table 4       Experimental vs         247 <i>n</i> -propyleyclohexane       429.90       424.59       Table 4       Experimental vs         248 <i>n</i> -propyleyclohexane       429.65       298.79       1       H_2O       37         251       Neopentyl glycol       483.00       496.79       1       H_2O       47         254 <i>o</i> -dichylbenzene       456.61       450.27       3       NH_3       24         255	236	<i>n</i> -pentane	309.23	300.04	290	Trans-1,4-dimeth	ylcycloh
238 <i>n</i> -pentylamine377.65380.12292 <i>Trans</i> -2-hexene239Propanol370.35352.65293 <i>Trans</i> -crotonoic act240 <i>n</i> -propionaldehyde321.15317.36294Trimethylamine241 <i>n</i> -propyl acetate374.65380.81295Valeraldehyde242 <i>n</i> -propyl chloride319.67309.94296Valerci acid243 <i>n</i> -propyl formate395.65405.66298Vinyl acetate244 <i>n</i> -propyl propionate395.65405.66298Vinyl acetate245 <i>n</i> -propyl benzene432.39428.72428.72247 <i>n</i> -propylcyclohexane429.90424.59Table 4Experimental vs inorganics using Eq. (9) wi248 <i>n</i> -propylcyclopentane404.11400.72NoCompound $T_{ex}$ 250Neopentane282.65298.791H <sub>2</sub> O37251Neopentyl glycol483.00496.791H <sub>2</sub> O37252 <i>o</i> -cresol464.15479.633NH <sub>3</sub> 24254 <i>o</i> -ditchlyblenzene456.61450.274N <sub>2</sub> H <sub>4</sub> 38255 <i>o</i> -ethlytoluene438.33429.095NH <sub>2</sub> OH33256 <i>o</i> -toluidine473.55449.397CH <sub>3</sub> F19258 <i>p</i> -cresol475.13474.149HCN29260 <i>p</i> -ditchlybenzene450.28450.219HF29261<	237	<i>n</i> -pentyl formate	406.60	405.24	291	Trans-2-butene	
239Propanol370.35352.65293Trans-crotonoic act240 $n$ -propionaldehyde321.15317.36294Trimethylamine241 $n$ -propyl acetate374.65380.81295Valeraldehyde242 $n$ -propyl chloride319.67309.94296Valeric acid243 $n$ -propyl formate353.97353.13297Valeronitrile244 $n$ -propyl propionate395.65405.66298Vinyl acetate245 $n$ -propyl mine321.65322.04247246 $n$ -propylepropionate404.11400.72428.72247 $n$ -propylcyclohexane429.90424.59428.72248 $n$ -propylcyclopentane404.11400.72420.92249 $n$ -tetradecane526.73512.20NoCompound250Neopentane282.65298.791H_2O251 $n$ -citchlorobenzene453.57465.944N_2H_4253 $o$ -dichlorobenzene456.61450.274N_2H_4254 $o$ -dichlylbenzene475.13474.148CH_3NH_2256 $p$ -cluidine473.55449.397CH_3F19258 $p$ -cresol475.13474.148CH_3NH_226260 $p$ -dichylbenzene450.28450.219HF29261 $p$ -diisopropylbenzene456.61429.277CH_3F19256 $o$ -ctulidine <td>238</td> <td><i>n</i>-pentylamine</td> <td>377.65</td> <td>380.12</td> <td>292</td> <td>Trans-2-hexene</td> <td></td>	238	<i>n</i> -pentylamine	377.65	380.12	292	Trans-2-hexene	
240 <i>n</i> -propionaldehyde       321.15       317.36       294       Trimethylamine         241 <i>n</i> -propyl acetate       374.65       380.81       295       Valeraldehyde         242 <i>n</i> -propyl chloride       319.67       309.94       296       Valeric acid         243 <i>n</i> -propyl formate       395.65       405.66       298       Vialeronitrile         244 <i>n</i> -propyl propionate       395.65       405.66       298       Vinyl acetate         245 <i>n</i> -propyl propionate       321.65       322.04       247 <i>n</i> -propylophenzene       432.39       428.72         247 <i>n</i> -propylcyclohexane       429.90       424.59       Table 4       Experimental vs inorganics using Eq. (9) wi         248 <i>n</i> -propylcyclopentane       404.11       400.72       No       Compound $T_{ex}$ 250       Neopentyl glycol       483.00       496.79       1       H_2O       37         251       Neopentyl glycol       483.00       496.79       2       H_2O_2       42         254 <i>o</i> -dichlorobenzene       453.57       465.94       4       N <sub>2</sub> H <sub>4</sub> 38         255 <i>o</i> -ethyltoluene       438.33       429.09 <td>239</td> <td>Propanol</td> <td>370.35</td> <td>352.65</td> <td>293</td> <td>Trans-crotonoic a</td> <td>acid</td>	239	Propanol	370.35	352.65	293	Trans-crotonoic a	acid
241 <i>n</i> -propyl acetate       374.65       380.81       295       Valeraldehyde         242 <i>n</i> -propyl chloride       319.67       309.94       296       Valerci acid         243 <i>n</i> -propyl formate       353.97       353.13       297       Valeronitrile         244 <i>n</i> -propyl propionate       395.65       405.66       298       Vinyl acetate         245 <i>n</i> -propyl amine       321.65       322.04       247 <i>n</i> -propylopcolenzene       432.39       428.72         247 <i>n</i> -propylcyclopentane       404.11       400.72       Table 4 Experimental vs       inorganics using Eq. (9) wi         248 <i>n</i> -propylcyclopentane       282.65       298.79       1       H <sub>2</sub> O       37         250       Neopentyl glycol       483.00       496.79       1       H <sub>2</sub> O       37         252 <i>o</i> -cresol       464.15       479.63       3       NH <sub>3</sub> 24         254 <i>o</i> -dichlorobenzene       453.57       465.94       4       N <sub>2</sub> H <sub>4</sub> 38         255 <i>o</i> -ethyltoluene       438.33       429.09       6       HCN       29         257 <i>o</i> -xylene       417.58       406.39	240	n-propionaldehyde	321.15	317.36	294	Trimethylamine	
242 <i>n</i> -propyl chloride319.67309.94296Valeric acid243 <i>n</i> -propyl formate353.97353.13297Valeronitrile244 <i>n</i> -propyl propionate395.65405.66298Vinyl acetate245 <i>n</i> -propyl amine321.65322.04246246 <i>n</i> -propylbenzene432.39428.72247247 <i>n</i> -propylcyclohexane429.90424.59Table 4248 <i>n</i> -propylcyclopentane404.11400.72Mo249 <i>n</i> -tetradecane526.73512.20No250Neopentyl glycol483.00496.791251Neopentyl glycol464.15479.632252 <i>o</i> -cresol464.15479.632253 <i>o</i> -dichlorobenzene453.57465.943254 <i>o</i> -dichylbenzene456.61450.274255 <i>o</i> -ethyltoluene438.33429.095256 <i>o</i> -stylene417.58406.397258 <i>p</i> -cresol475.13474.148260 <i>p</i> -diethylbenzene456.94450.43261 <i>p</i> -diisopropylbenzene456.94450.43262 <i>p</i> -ethyltoluene435.16429.27263 <i>p</i> -hydroquinone558.15550.36264 <i>p</i> -tuluidine473.40454.67265 <i>p</i> -xylene411.51406.48266Phenol454.99457.86276Neperiptor<	241	<i>n</i> -propyl acetate	374.65	380.81	295	Valeraldehyde	
243 <i>n</i> -propyl formate353.97353.13297Valeronitrile244 <i>n</i> -propyl propionate395.65405.66298Vinyl acetate245 <i>n</i> -propyl amine321.65322.04246246 <i>n</i> -propylbenzene432.39428.72247247 <i>n</i> -propylcyclohexane429.90424.59Table 4 Experimental vs248 <i>n</i> -propylcyclopentane404.11400.72No249 <i>n</i> -tetradecane526.73512.20NoCompound $T_{er}$ 250Neopentyl glycol483.00496.791H <sub>2</sub> O251Neopentyl glycol483.00496.792H <sub>2</sub> O <sub>2</sub> 42253 <i>o</i> -dichlorobenzene453.57465.943NH <sub>3</sub> 24254 <i>o</i> -diethylbenzene456.61450.275NH <sub>2</sub> OH33256 <i>o</i> -toluidine473.55449.396HCN29257 <i>o</i> -xylene417.58406.397CH <sub>3</sub> F19258 <i>p</i> -cresol475.13474.148CH <sub>3</sub> NH <sub>2</sub> 26259 <i>p</i> -bydroquinone558.15550.36(R <sup>2</sup> =0.902, s=25.04 K, F=7NDescriptor263 <i>p</i> -hydroquinone558.15550.36(R <sup>2</sup> =0.902, s=25.04 K, F=7NDescriptor264 <i>p</i> -tuluidine473.40454.67NDescriptor265 <i>p</i> -xylene411.51406.481Intercept	242	<i>n</i> -propyl chloride	319.67	309.94	296	Valeric acid	
244 <i>n</i> -propyl propionate395.65405.66298Vinyl acetate245 <i>n</i> -propyl amine321.65322.047246 <i>n</i> -propylbenzene432.39428.727247 <i>n</i> -propylcyclohexane429.90424.597248 <i>n</i> -propylcyclopentane404.11400.72400.72249 <i>n</i> -tetradecane526.73512.205250Neopentane282.65298.791251Neopentyl glycol483.00496.792252 <i>o</i> -cresol464.15479.633253 <i>o</i> -dichlorobenzene453.57465.943254 <i>o</i> -diethylbenzene456.61450.274255 <i>o</i> -ethyltoluene438.33429.095257 <i>o</i> -xylene417.58406.397258 <i>p</i> -cresol475.13474.14259 <i>p</i> -cymene450.28450.21260 <i>p</i> -diethylbenzene435.16429.27261 <i>p</i> -diisopropylbenzene483.65488.64262 <i>p</i> -ethyltoluene435.16429.27263 <i>p</i> -hydroquinone558.15550.36264 <i>p</i> -tuluidine473.40454.67265 <i>p</i> -xylene411.51406.48266Phenol454.99457.86277 <i>p</i> -discriptor	243	<i>n</i> -propyl formate	353.97	353.13	297	Valeronitrile	
245 <i>n</i> -propyl amine321.65322.04246 <i>n</i> -propylbenzene432.39428.72247 <i>n</i> -propylcyclohexane429.90424.59248 <i>n</i> -propylcyclopentane404.11400.72249 <i>n</i> -tetradecane526.73512.20250Neopentane282.65298.79251Neopentyl glycol483.00496.79252 <i>o</i> -cresol464.15479.63253 <i>o</i> -dichlorobenzene453.57465.94254 <i>o</i> -diethylbenzene456.61450.27255 <i>o</i> -ethyltoluene438.33429.09256 <i>o</i> -toluidine473.55449.39257 <i>o</i> -xylene417.58406.39258 <i>p</i> -cresol475.13474.14259 <i>p</i> -cymene456.94450.21260 <i>p</i> -diithylbenzene438.65488.64262 <i>p</i> -ethyltoluene436.55488.64262 <i>p</i> -ethyltoluene435.16429.27263 <i>p</i> -hydroquinone558.15550.36264 <i>p</i> -tuluidine473.40454.67265 <i>p</i> -xylene411.51406.48266 <i>P</i> henol454.99457.86266Phenol454.99457.86	244	<i>n</i> -propyl propionate	395.65	405.66	298	Vinyl acetate	
246 <i>n</i> -propylbenzene432.39428.72247 <i>n</i> -propylcyclohexane429.90424.59Table 4 Experimental vs. inorganics using Eq. (9) wi248 <i>n</i> -propylcyclopentane404.11400.72No249 <i>n</i> -tetradecane526.73512.20No250Neopentane282.65298.791 $H_2O$ 251Neopentyl glycol483.00496.792 $H_2O_2$ 42253 <i>o</i> -dichlorobenzene453.57465.943NH324254 <i>o</i> -diethylbenzene456.61450.274 $N_2H_4$ 38255 <i>o</i> -ethyltoluene438.33429.095NH2OH33256 <i>o</i> -toluidine473.55449.396HCN29257 <i>o</i> -xylene417.58406.397CH_3F19258 <i>p</i> -cresol475.13474.148CH_3NH226260 <i>p</i> -diitsopropylbenzene456.94450.28450.219HF29261 <i>p</i> -diisopropylbenzene438.65488.64262 <i>p</i> -ethyltoluene435.16429.277Table 5The QSPR equation of the properties of the properti	245	<i>n</i> -propyl amine	321.65	322.04			
247n-propylcyclohexane429.90424.59Table 4Experimental vs inorganics using Eq. (9) wi248n-propylcyclopentane404.11400.72NoCompound $T_{ey}$ 249n-tetradecane526.73512.20NoCompound $T_{ey}$ 250Neopentane282.65298.791 $H_2O$ 37251Neopentyl glycol483.00496.792 $H_2O_2$ 42253o-cresol464.15479.633 $NH_3$ 24254o-diethylbenzene456.61450.274 $N_2H_4$ 38255o-ethyltoluene438.33429.095 $NH_2OH$ 33256o-toluidine473.55449.396HCN29257o-xylene417.58406.397CH_3F19258p-cresol475.13474.148CH_3NH_226259p-cymene456.94450.439HF29260p-diethylbenzene456.54488.649HF29261p-diisopropylbenzene483.65488.64 $(R^2=0.902, s=25.04$ K, $F=7$ 263p-hydroquinone558.15550.36 $(R^2=0.902, s=25.04$ K, $F=7$ 264p-tuluidine473.40454.67NDescriptor265p-xylene411.51406.48NDescriptor266Phenol454.99457.861Intercept	246	<i>n</i> -propylbenzene	432.39	428.72			
248 <i>n</i> -propylcyclopentane404.11400.72morganics using Eq. (9) with No249 <i>n</i> -tetradecane526.73512.20NoCompound $T_{ex}$ 250Neopentane282.65298.791H <sub>2</sub> O37251Neopentyl glycol483.00496.792H <sub>2</sub> O <sub>2</sub> 42253 <i>o</i> -dichlorobenzene453.57465.943NH <sub>3</sub> 24254 <i>o</i> -diethylbenzene456.61450.274N <sub>2</sub> H <sub>4</sub> 38255 <i>o</i> -ethyltoluene438.33429.096HCN29257 <i>o</i> -xylene417.58406.397CH <sub>3</sub> F19258 <i>p</i> -cresol475.13474.148CH <sub>3</sub> NH <sub>2</sub> 26259 <i>p</i> -cymene456.94450.439HF29260 <i>p</i> -ditethylbenzene483.65488.649HF29261 <i>p</i> -ditopropylbenzene435.16429.27Table 5The QSPR equation organic compounds obtained ( $R^2$ =0.902, $s$ =25.04 K, $F$ =7263 <i>p</i> -hydroquinone558.15550.36( $R^2$ =0.902, $s$ =25.04 K, $F$ =7264 <i>p</i> -tuluidine473.40454.67NDescriptor265 <i>p</i> -xylene411.51406.48NDescriptor266Phenol454.99457.861Intercept	247	n-propylcyclohexane	429.90	424.59	Table	4 Experimental	vs calcu
249 <i>n</i> -tetradecane526.73512.20NoCompound $T_{ex}$ 250Neopentane282.65298.791 $H_2O$ 37251Neopentyl glycol483.00496.792 $H_2O_2$ 42252 <i>o</i> -cresol464.15479.633NH <sub>3</sub> 24253 <i>o</i> -dichlorobenzene453.57465.943NH <sub>3</sub> 24254 <i>o</i> -diethylbenzene456.61450.274N <sub>2</sub> H <sub>4</sub> 38255 <i>o</i> -ethyltoluene438.33429.095NH <sub>2</sub> OH33256 <i>o</i> -toluidine473.55449.396HCN29257 <i>o</i> -xylene417.58406.397CH <sub>3</sub> F19258 <i>p</i> -cresol475.13474.148CH <sub>3</sub> NH <sub>2</sub> 26260 <i>p</i> -diethylbenzene456.94450.28450.219HF29260 <i>p</i> -diethylbenzene435.16429.27Table 5The QSPR equation263 <i>p</i> -hydroquinone558.15550.36 $(R^2=0.902, s=25.04$ K, <i>F=7</i> NDescriptor264 <i>p</i> -tuluidine473.40454.67NDescriptor1Intercept266Phenol454.99457.861Intercept1Intercept	248	<i>n</i> -propylcyclopentane	404.11	400.72	inorga	inics using Eq. (9)	with new
250Neopentane $282.65$ $298.79$ $1$ $H_2O$ $37$ 251Neopentyl glycol $483.00$ $496.79$ $1$ $H_2O_2$ $42$ 252 $o$ -cresol $464.15$ $479.63$ $3$ $NH_3$ $24$ 253 $o$ -dichlorobenzene $453.57$ $465.94$ $3$ $NH_3$ $24$ 254 $o$ -dicthylbenzene $456.61$ $450.27$ $4$ $N_2H_4$ $38$ 255 $o$ -ethyltoluene $438.33$ $429.09$ $5$ $NH_2OH$ $33$ 256 $o$ -toluidine $473.55$ $449.39$ $6$ $HCN$ $29$ 257 $o$ -xylene $417.58$ $406.39$ $7$ $CH_3F$ $19$ 258 $p$ -cresol $475.13$ $474.14$ $8$ $CH_3NH_2$ $26$ 259 $p$ -cymene $450.28$ $450.21$ $9$ $HF$ $29$ 260 $p$ -dithylbenzene $435.16$ $429.27$ $7$ $Table 5$ $The QSPR equation or granic compounds obtainee263p-hydroquinone558.15550.36(R^2=0.902, s=25.04 \text{ K}, F=7)265p-xylene411.51406.48NDescriptor266Phenol454.99457.861Intercept$	249	<i>n</i> -tetradecane	526.73	512.20	No	Compound	T <sub>exp</sub> , K
251Neopentyl glycol483.00496.791 $H_2O$ 37252 $o$ -cresol464.15479.632 $H_2O_2$ 42253 $o$ -dichlorobenzene453.57465.943NH324254 $o$ -diethylbenzene456.61450.274 $N_2H_4$ 38255 $o$ -ethyltoluene438.33429.095NH <sub>2</sub> OH33256 $o$ -toluidine473.55449.396HCN29257 $o$ -xylene417.58406.397CH <sub>3</sub> F19258 $p$ -cresol475.13474.148CH <sub>3</sub> NH <sub>2</sub> 26259 $p$ -cymene450.28450.219HF29260 $p$ -diethylbenzene483.65488.649HF29261 $p$ -diisopropylbenzene435.16429.27Table 5The QSPR equation or granic compounds obtainee263 $p$ -hydroquinone558.15550.36 $(R^2=0.902, s=25.04 \text{ K}, F=7)$ 264 $p$ -tuluidine473.40454.67NDescriptor265 $p$ -xylene411.51406.48NDescriptor266Phenol454.99457.861Intercept	250	Neopentane	282.65	298.79	1	шо	272
252 $o$ -cresol464.15479.63 $2$ $H_2O_2$ 42253 $o$ -dichlorobenzene453.57465.943NH324254 $o$ -diethylbenzene456.61450.274N $_2H_4$ 38255 $o$ -ethyltoluene438.33429.095NH $_2OH$ 33256 $o$ -toluidine473.55449.396HCN29257 $o$ -xylene417.58406.397CH $_3F$ 19258 $p$ -cresol475.13474.148CH $_3NH_2$ 26259 $p$ -cymene450.28450.219HF29260 $p$ -diethylbenzene483.65488.649HF29261 $p$ -diisopropylbenzene483.65488.64262 $p$ -ethyltoluene558.15550.36 $(R^2=0.902, s=25.04$ K, $F=7$ 263 $p$ -hydroquinone558.15550.36 $(R^2=0.902, s=25.04$ K, $F=7$ $N$ Descriptor265 $p$ -xylene411.51406.48 $N$ Descriptor266Phenol454.99457.86 $1$ Intercept	251	Neopentyl glycol	483.00	496.79	1	H <sub>2</sub> O	373
253 $o$ -dichlorobenzene453.57465.94 $3$ $NH_3$ 24254 $o$ -diethylbenzene456.61450.274 $N_2H_4$ 38255 $o$ -ethyltoluene438.33429.095 $NH_2OH$ 33256 $o$ -toluidine473.55449.396HCN29257 $o$ -xylene417.58406.397 $CH_3F$ 19258 $p$ -cresol475.13474.148 $CH_3NH_2$ 26259 $p$ -cymene450.28450.219HF29260 $p$ -diethylbenzene436.55488.649HF29261 $p$ -diisopropylbenzene435.16429.27Table 5The QSPR equation or granic compounds obtained or granic compounds obtai	252	o-cresol	464.15	479.63	2	$H_2O_2$	425
254 $o$ -diethylbenzene456.61450.274 $N_2H_4$ 38255 $o$ -ethyltoluene438.33429.095 $NH_2OH$ 33256 $o$ -toluidine473.55449.396 $HCN$ 29257 $o$ -xylene417.58406.397 $CH_3F$ 19258 $p$ -cresol475.13474.148 $CH_3NH_2$ 26259 $p$ -cymene450.28450.219 $HF$ 29260 $p$ -diethylbenzene436.5488.649 $HF$ 29261 $p$ -diisopropylbenzene435.16429.27Table 5The QSPR equation of the second solution of	253	o-dichlorobenzene	453.57	465.94	3	NH <sub>3</sub>	240
255 $o$ -ethyltoluene438.33429.095 $NH_2OH$ 33256 $o$ -toluidine473.55449.396HCN29257 $o$ -xylene417.58406.397 $CH_3F$ 19258 $p$ -cresol475.13474.148 $CH_3NH_2$ 26259 $p$ -cymene450.28450.219HF29260 $p$ -diethylbenzene456.94450.439HF29261 $p$ -diisopropylbenzene483.65488.649HF29263 $p$ -hydroquinone558.15550.36 $(R^2=0.902, s=25.04 \text{ K}, F=7)$ 264 $p$ -tuluidine473.40454.67NDescriptor265 $p$ -xylene411.51406.481Intercept	254	o-diethylbenzene	456.61	450.27	4	$N_2H_4$	387
256 $o$ -toluidine473.55449.396HCN29257 $o$ -xylene417.58406.397CH <sub>3</sub> F19258 $p$ -cresol475.13474.148CH <sub>3</sub> NH <sub>2</sub> 26259 $p$ -cymene450.28450.219HF29260 $p$ -diethylbenzene456.94450.439HF29261 $p$ -diisopropylbenzene483.65488.649HF29262 $p$ -ethyltoluene435.16429.27Table 5The QSPR equation of the transition of transition of the	255	o-ethyltoluene	438.33	429.09	5	NH <sub>2</sub> OH	330
257 $o$ -xylene417.58406.397 $CH_3F$ 19258 $p$ -cresol475.13474.148 $CH_3NH_2$ 26259 $p$ -cymene450.28450.219HF29260 $p$ -diethylbenzene456.94450.439HF29261 $p$ -diisopropylbenzene483.65488.649HF29262 $p$ -ethyltoluene435.16429.27Table 5The QSPR equation or granic compounds obtainee263 $p$ -hydroquinone558.15550.36 $(R^2=0.902, s=25.04 \text{ K}, F=7)$ 264 $p$ -tuluidine473.40454.67NDescriptor265 $p$ -xylene411.51406.481Intercept	256	o-toluidine	473.55	449.39	6	HCN	299
258p-cresol475.13474.148 $CH_3NH_2$ 26259p-cymene450.28450.219HF29260p-diethylbenzene456.94450.439HF29261p-diisopropylbenzene483.65488.64488.64450.279HF29263p-tydroquinone558.15550.36Table 5The QSPR equation or ganic compounds obtained or ganic compoun	257	o-xylene	417.58	406.39	7	CH <sub>3</sub> F	195
259 $p$ -cymene450.28450.219HF29260 $p$ -diethylbenzene456.94450.4320261 $p$ -diisopropylbenzene483.65488.64262 $p$ -ethyltoluene435.16429.27Table 5263 $p$ -hydroquinone558.15550.36 $(R^2=0.902, s=25.04 \text{ K}, F=7)$ 264 $p$ -tuluidine473.40454.67NDescriptor265 $p$ -xylene411.51406.481Intercept	258	<i>p</i> -cresol	475.13	474.14	8	CH <sub>3</sub> NH <sub>2</sub>	267
260p-diethylbenzene456.94450.43261p-diisopropylbenzene483.65488.64262p-ethyltoluene435.16429.27263p-hydroquinone558.15550.36264p-tuluidine473.40454.67265p-xylene411.51406.48266Phenol454.99457.86	259	<i>p</i> -cymene	450.28	450.21	9	HF	293
261p-diisopropylbenzene483.65488.64262p-ethyltoluene435.16429.27263p-hydroquinone558.15550.36264p-tuluidine473.40454.67265p-xylene411.51406.48266Phenol454.99457.86	260	<i>p</i> -diethylbenzene	456.94	450.43			
262 $p$ -ethyltoluene       435.16       429.27       Table 5       The QSPR equations         263 $p$ -hydroquinone       558.15       550.36       organic compounds obtained         264 $p$ -tuluidine       473.40       454.67 $R^2$ =0.902, $s$ =25.04 K, $F$ =7         265 $p$ -xylene       411.51       406.48       N       Descriptor         266       Phenol       454.99       457.86       1       Intercept	261	<i>p</i> -diisopropylbenzene	483.65	488.64			
263 $p$ -hydroquinone       558.15       550.36       organic compounds obtained         264 $p$ -tuluidine       473.40       454.67 $(R^2=0.902, s=25.04 \text{ K}, F=7)$ 265 $p$ -xylene       411.51       406.48       N       Descriptor         266       Phenol       454.99       457.86       1       Intercept	262	<i>p</i> -ethyltoluene	435.16	429.27	Table	5 The QSPR equ	ation for
264 $p$ -tuluidine       473.40       454.67 $(R^{-2}=0.902, s=25.04 \text{ K}, F=7)$ 265 $p$ -xylene       411.51       406.48 $N$ Descriptor         266       Phenol       454.99       457.86       1       Intercept	263	<i>p</i> -hydroquinone	558.15	550.36	organi	ic compounds obtain	ned with
265 <i>p</i> -xylene         411.51         406.48 <i>N</i> Descriptor           266         Phenol         454.99         457.86         1         Intercept	264	<i>p</i> -tuluidine	473.40	454.67	$(R^2=0$	.902, <i>s</i> =25.04 K, <i>F</i>	=/42./3
266 Phenol 454.99 457.86 1 Intercept	265	<i>p</i> -xylene	411.51	406.48	N	Descriptor	Х
I Intercept	266	Phenol	454.99	457.86	1	<b>T</b> · · ·	
267 Piperidine 379.55 403.52	267	Piperidine	379.55	403.52	1	Intercept	
268 Propane $231.11 \ 214.55 \$	268	Propane	231.11	214.55	2	GI	

No	Compound	$T_{\rm exp}$ , K	$T_{\text{calc}}, \mathbf{K}$
.69	Propionic acid	414.32	419.14
270	Propionitrile	370.50	319.73
271	Propylene	225.43	216.03
272	Pyridine	388.41	361.34
273	Quinoline	510.75	522.79
274	Sec-butyl acetate	385.15	405.41
275	Sec-butyl alcohol	372.70	374.97
276	Sec-butyl chloride	341.25	340.18
277	Sec-butyl amine	336.15	340.01
278	Sec-butyl benzene	446.48	449.64
.79	Stearic acid	648.35	645.59
280	Styrene	418.31	406.43
281	Tert-butyl acetate	369.15	405.04
282	Tert-buty alcohol	355.57	368.90
283	Tert-butyl chloride	323.75	338.03
284	Tert-butyl amine	317.55	342.45
285	Tert-butylbenzene	442.30	449.01
286	Tetrahydrofuran	338.00	328.78
287	Toluene	383.78	381.00
288	Trans-1,2-dimethylcyclohexane	396.58	401.06
.89	Trans-1,3-dimethylcyclohexane	397.61	401.17
.90	Trans-1,4-dimethylcyclohexane	392.51	401.19
.91	Trans-2-butene	274.03	263.84
.92	Trans-2-hexene	341.02	334.94
.93	Trans-crotonoic acid	458.15	443.28
.94	Trimethylamine	276.02	315.52
.95	Valeraldehyde	376.15	373.82
.96	Valeric acid	458.65	460.87
.97	Valeronitrile	414.45	374.04
.98	Vinyl acetate	345.65	354.95

ulated boiling points for NINE w AM1 parameters

No	Compound	$T_{\rm exp}$ , K	$T_{\text{calc}}, \mathbf{K}$	$F=T_{exp}-T_{calc}$
1	H <sub>2</sub> O	373	369.17	3.83
2	$H_2O_2$	425	436.24	-11.24
3	NH <sub>3</sub>	240	256.73	-16.73
4	$N_2H_4$	387	357.04	29.96
5	NH <sub>2</sub> OH	330	343.62	-13.62
6	HCN	299	308.84	-9.84
7	CH <sub>3</sub> F	195	194.31	0.69
8	CH <sub>3</sub> NH <sub>2</sub>	267	262.28	4.72
9	HF	293	280.77	12.23

r the critical temperatures of 165 the re-optimized AM1 parameters

N	Descriptor	$X + \Delta X$	<i>t</i> -test
1	Intercept	-173±18.3	-6.40
2 3	$G_{\rm I}^{\rm ASS}$ HASA(2)	81±2.2 12±0.76	36.81 16.71

Table 6 The experimental vs. predicted critical temperatures for 165 organic compounds (according to the QSPR model from Table 5)

Number	Compound	$T_{\rm exp}$ , K	$T_{\text{cale}}, \mathrm{K}$	Number	Compound	$T_{\rm exp},  {\rm K}$	$T_{\text{calc}}, \mathrm{K}$
1	3-chloropropene	514.2	479.5	83	Ethylcyclopentane	569.5	558.2
2	Propylene	364.8	363.9	84	2,3-dimethylpentane	537.4	541.5
3	1,2-dichloropropene	545.1	572.1	85	<i>n</i> -heptane	540.3	542.7
4	Ethylformate	508.4	493.9	86	2-methylhexane	530.4	542.2
5	Methyl acetate	506.8	494.6	87	3-methylhexane	535.3	542.0
6	Propionic acid	604.0	561.2	88	Ethylbenzene	617.2	595.4
7	<i>n</i> -propyl chloride	503.2	478.4	89	<i>m</i> -xylene	617.1	596.1
8	Propane	369.8	362.1	90	<i>p</i> -xylene	616.3	596.1
9	Methyl ethyl ether	437.8	437.6	91	2,6-xylenol	701.1	691.0
10	<i>n</i> -propanol	536.7	500.4	92	N,N-dimethylaniline	687.2	663.6
11	Methylal	480.6	498.1	93	cis-1,2-dimethylcyclohexane	606.2	589.6
12	Isopropylamine	471.9	476.3	94	trans-1,2-dimethylcyclohexane	596.2	589.5
13	<i>n</i> -propylamine	497.0	484.4	95	cis-1,3-dimethylcyclohexane	591.2	589.7
14	Trimethylamine	433.3	476.9	96	trans-1,3-dimethylcyclohexane	598.0	589.7
15	1,3-butadiene	425.4	421.9	97	trans-1,4-dimethylcyclohexane	590.2	589.7
16	Butyronitrile	582.3	575.3	98	ethylcyclohexane	609.2	589.8
17	1-butene	419.6	420.6	99	isobutyl isobutyrate	602.0	648.4
18	cis-2-butene	435.6	422.4	100	2,3-dimethylhexane	563.4	573.9
19	trans-2-butene	428.6	422.2	101	2-methyl-3-ethylpentane	567.0	573.8
20	Isobutene	417.9	421.5	102	<i>n</i> -octane	568.8	575.0
21	Methyl ethyl ketone	535.5	553.7	103	2,2,3-trimethylpentane	563.5	572.6
22	Tetrahydrofuran	540.2	501.4	104	2,2,4-trimethylpentane	544.0	573.0
23	<i>n</i> -butyric acid	628.0	599.4	105	2,3,3-trimethylpentane	573.0	572.8
24	Ethyl acetate	523.3	531.5	106	2-ethyl-1-hexanol	640.0	670.3
25	Isobutyric acid	609.2	600.0	107	Quinoline	782.2	731.9
26	Methyl proprionate	530.6	531.6	108	Cumene	631.2	622.9
27	<i>n</i> -propyl formate	538.0	531.1	109	o-ethyltoluene	651.2	623.8
28	<i>n</i> -butane	425.2	419.3	110	<i>p</i> -ethyltoluene	640.2	624.0
29	Isobutane	408.1	418.7	111	Mesitylene	637.4	624.6
30	Butanol	562.9	539.9	112	<i>n</i> -propylbenzene	638.4	623.3
31	sec-butyl alcohol	536.0	537.0	113	1,2,3-trimethylbenzene	664.5	624.2
32	tert-butyl alcohol	506.2	538.4	114	1,2,4-trimethylbenzene	649.1	624.4
33	Diethyl ether	466.7	481.7	115	<i>n</i> -propylcyclohexane	639.2	618.2
34	Isobutanol	547.7	535.5	116	3,3-diethylpentane	610.1	602.9
35	<i>n</i> -butylamine	531.9	529.6	117	<i>n</i> -nonane	595.7	604.5
36	Diethylamine	496.6	516.1	118	2,2,3,3-tetramethylpentane	610.9	601.3
37	Pyridine	620.0	604.5	119	1,2,3,4-tetrahydronaphthalene	720.2	662.6
38	Cyclopentane	511.8	486.3	120	<i>n</i> -butylbenzene	660.6	649.3
39	1-pentane	464.8	467.5	121	<i>p</i> -cymene	653.2	649.5
40	Diethyl ketone	561.0	582.5	122	Isobutylbenzene	650.2	649.0
41	2-pentanone	561.1	595.4	123	<i>n</i> -decane	618.2	631.8
42	Ethyl propionate	546.0	564.7	124	<i>n</i> -tetradecane	692.4	725.1
43	Isobutyl formate	551.4	563.8	125	<i>n</i> -octadecane	745.3	801.3
44	n-propyl acetate	549.4	564.9	126	<i>n</i> -nonadecane	755.9	818.5
45	Valeric acid	651.0	632.2	127	sec-butylchloride	520.6	515.3
46	Isopentane	460.4	465.7	128	Methyl isopropyl ether	464.5	481.5
47	Neopentane	433.8	464.8	129	sec-butylamine	514.3	525.4
48	<i>n</i> -pentane	469.7	466.3	130	tert-butylamine	483.9	518.5
49	2-methyl-2-butanol	545.2	575.4	131	2-methyl-1-butene	465.0	468.1
50	3-methyl-1-butanol	579.5	584.3	132	2-methyl-2-butene	471.0	469.4
51	1-pentanol	586.2	584.9	133	3-methyl-1-butene	450.4	466.9
52	Bromobenzene	670.2	631.7	134	Methyl isopropyl ketone	553.0	593.4
53	Chlorobenzene	632.4	606.9	135	Methyl <i>n</i> -butyrate	554.5	565
54	Benzene	562.2	531.1	136	Piperidine	594.1	575.7

Table 6 (continued)

Number	Compound	$T_{\rm exp}$ , K	$T_{\text{calc}}, \mathbf{K}$	Number	Compound	$T_{\rm exp},  {\rm K}$	$T_{\text{calc}}, \mathbf{K}$
55	Phenol	694.3	642.4	137	Ethyl propyl ether	500.2	520.4
56	Aniline	699.0	622.0	138	Methyl tert-butyl ether	497.1	519.5
57	2-methylpyridine	621.0	636.2	139	3-methylpyridine	645.0	643.9
58	Cyclohexene	560.4	527.4	140	1,5-hexadiene	507.0	508.8
59	Cyclohexanone	629.2	651.3	141	Hexanenitrile	622.1	651.6
60	Cyclohexane	553.5	525.5	142	3-hexanone	582.8	618.9
61	1-hexene	504.0	507.8	143	Ethyl isobutyrate	553.2	594.7
62	Methylcyclopentane	532.8	524.2	144	<i>n</i> -propyl propionate	578.0	595.1
63	Cyclohexanol	625.2	631.1	145	1-hexanol	611.4	618.9
64	2-hexanone	587.1	627.9	146	2-hexanol	586.2	616.4
65	Methyl isobutyl ketone	571.4	629.2	147	4-methyl-2-pentanol	574.4	617.4
66	Ethyl <i>n</i> -butyrate	571.0	595.2	148	Acetone	508.2	517.5
67	Isobutyl acetate	561.0	594.9	149	2-propanol	508.3	495.9
68	2,2-dimethylbutane	488.8	505.3	150	Ethyl vinyl ether	475.2	483.7
69	2,3-dimethylbutane	500.0	505.6	151	Isovaleric acid	634.0	634.1
70	<i>n</i> -hexane	507.4	506.8	152	<i>n</i> -butyl acetate	579.2	595.2
71	2-methylpentane	497.5	506.3	153	<i>p</i> -cresol	704.7	673.0
72	3-methylpentane	504.4	506.1	154	<i>p</i> -toluidine	693.2	657.4
73	Diisopropyl ether	500.1	553.9	155	1-heptene	537.3	543.5
74	Di-n-propyl ether	530.6	554.8	156	Methylcyclohexane	572.2	559.1
75	Diisopropylamine	523.1	585.0	157	2,2,3-trimethylbutane	531.2	540.5
76	Di-n-propylamine	555.8	583.9	158	o-xylene	630.4	596.0
77	Benzaldehyde	695.0	688.2	159	1-octene	578.2	575.8
78	Toluene	591.8	565.1	160	<i>m</i> -methyltoluene	637.2	596.1
79	<i>m</i> -cresol	705.9	678.0	161	<i>p</i> -diethylbenzene	658.0	649.9
80	o-cresol	697.6	676.7	162	1-decene	617.1	632.5
81	<i>m</i> -toluidine	709.2	654.3	163	Propionitrile	564.4	531.0
82	o-toluidine	694.2	654.5	164	4-methylpyridine	646.2	637.7
				165	n-pentyl formate	576.0	594.6

**Fig. 2** The predicted vs experimental critical temperatures according to the best two-descriptor equation (Table 5) and new AM1 parameters



### Conclusions

The original AM1 quantum-chemical parameterization was improved to be more adequate for developing molecular descriptors and the related QSPR models in the liquid phase. A nonlinear optimization technique based on the Levenberg– Marquardt algorithm was used to optimize 17 parameters for the core–core repulsion function and one-electron resonance integrals for H, C, O, Cl, N and Br atoms. The results of the QSPR treatment of normal boiling points demonstrate that the new parameters describe the intermolecular interactions in liquid phase better. The descriptors appearing in the twoparameter QSPR equation are connected with dispersion and cavity formation processes, hydrogen bonding ability of the compounds and electrostatic intermolecular interactions in liquid media.

The new set of parameters also enabled the better prediction of the normal boiling points of nine simple inorganic compounds as compared to the original QSPR model.

The results obtained for the critical temperature of 165 organic compounds indicate that similar processes govern this property as of the boiling points. A two-descriptor original QSPR equation was improved by using the re-optimized parameters  $\alpha$ ,  $\beta_s$  and  $\beta_p$  from the treatment of boiling points. The fact that the new QSPR model involves two similar descriptors ( $\sqrt[3]{G_I}$  and HASA(2)) reveals that the dispersion and cavity formation phenomena as well as the hydrogen bonding ability are the most important interactions determining the critical temperatures of compounds. A more extensive validation of the new AM1 parameterization will be carried out on a series of other properties of compounds in the liquid phase (density, vapor pressure, distribution coefficients etc.).

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