

## A Linear Solvation Energy Relationship to Predict Vapor Pressure from Molecular Structure

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Pressões de vapor de líquidos orgânicos (em Pa a 298 K) correlacionam ( $R^2 = 0.986$ ) segundo a relação:

$$\log P_{\text{vap}} = 7.86 - 3.54 V - 1.17 E - 1.52 (S + \lambda) - 3.64 (\eta \times A \times B)$$

sendo  $V$ ,  $E$ ,  $S$ ,  $A$ , e  $B$  parâmetros empíricos para o volume molar, o índice de refração em excesso, a dipolaridade/polarizabilidade e a capacidade doadora e receptora de pontes de hidrogênio do soluto, respectivamente. O parâmetro  $\lambda$  ajusta o valor do termo em  $S$  para grupos funcionais específicos, enquanto considera diferenças na formação de pontes de hidrogênio entre classes distintas de líquidos puros. Essa relação linear de energia livre (LSER) é quimicamente razoável e permite a previsão da pressão de vapor de líquidos orgânicos a partir de parâmetros de soluto conhecidos ou estimados a partir de estrutura química. Esses resultados ilustram o potencial de uso de parâmetros de soluto para desenvolver LSERs para a previsão de propriedades de substâncias puras.

Vapor pressures (in Pa at 298 K) of organic liquids were found to correlate ( $R^2 = 0.986$ ) with empirical molecular parameters by the relationship:

$$\log P_{\text{vap}} = 7.86 - 3.54 V - 1.17 E - 1.52 (S + \lambda) - 3.64 (\eta \times A \times B)$$

where  $V$ ,  $E$ ,  $S$ ,  $A$ , and  $B$  are solute parameters developed by Abraham and coworkers representing, respectively, the characteristic volume, excess index of refraction, dipolarity/polarizability, and hydrogen bond donor and acceptor characteristics of the solute. The parameter  $\lambda$  provides for modulation of the  $S$  term for specific functional groups, such as those with strongly dipolar structures, while the parameter  $\eta$  takes into account differences in neat-liquid hydrogen bonding between classes of liquids. This linear free energy relationship (LSER), together with appropriate solute parameters taken from literature data or estimated from chemical structure, provides a convenient method for estimating the vapor pressure of pure organic liquids. This study also provides insight into the extent to which the LSER model may be extended to the prediction of properties of pure substances.

**Keywords:** LSER, vapor pressure, organic liquids, Abraham parameters, hydrogen bonding

### Introduction

The dispersal of organic liquids in the environment depends on their physical properties, especially their volatility and their solubility in water.<sup>1</sup> It is therefore of central importance in environmental studies to be able to predict these properties when experimental values are not available.<sup>2</sup> While these properties can sometimes be estimated on the basis of known physical constants, such as boiling point and heat of vaporization<sup>3</sup> or by computational methods,<sup>4</sup> it is particularly useful to have available methods to estimate these properties by inspection of molecular structure, without recourse to other experimental values or to computational

results. In the present work, we examine the potential advantages and limitations of employing a Linear Solvation Energy Relationship (LSER) approach for the estimation of the vapor pressure of organic liquids at 298 K.

As introduced by Kamlet and Taft<sup>5</sup> and subsequently developed by Abraham,<sup>6</sup> the LSER approach characterizes solvation effects in terms of nonspecific (orientation-independent) and hydrogen bonding interactions. Thus, a solvation property of interest ( $P$ ) for an organic solute is modeled by a linear free energy relationship of the form<sup>7</sup>

$$P = c + vV + eE + sS + aA + bB \quad (1)$$

where  $c$ ,  $v$ ,  $e$ ,  $s$ ,  $a$  and  $b$  are constants characteristic of the

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system being studied. The non-specific interactions are represented by  $V$ , the characteristic volume<sup>8</sup> of the molecule, which is taken to be a measure of cavitation and generalized dispersion interactions; by  $E$ , the excess molar refraction of the compound relative to that of an aliphatic hydrocarbon of the same molar volume, which is thought to indicate the importance of interactions of molecules through their pi- and  $n$ -electron pairs; and by  $S$ , a measure of the dipolarity/polarizability of the solute.<sup>9</sup> The specific interactions are incorporated through the  $A$  and  $B$  parameters, which respectively represent the sums of the hydrogen bond donor and hydrogen bond acceptor characteristics of the solute. This LSER approach has been used to develop predictive equations for a wide variety of chromatographic and phase transfer processes.<sup>10</sup>

The Abraham method was developed to model interactions of a set of solutes of diverse structure with a single solvent system or their transfer between two solvents or between a solvent and another phase. Recently, however, we began to explore the viability of the LSER approach for the estimation of physical properties of pure substances, including the work of interfacial adhesion of organic liquids with water<sup>11</sup> and the surface tension of organic liquids.<sup>12</sup> Along the same lines, Abraham has reported a correlation for the solubility of neat organic compounds in water,<sup>13</sup> and recently Bel'skii reported a correlation of vapor pressure along the lines of equation 1 but with an additional  $V^2$  term.<sup>9</sup>

All of the applications discussed in the preceding paragraph represent significant departures from the original Abraham model because for each compound the surrounding solvent molecules are different for each solute molecule in the neat liquid. In each of these cases a reasonable LSER was reported, however, suggesting that applying the Abraham method to pure liquids has some validity. It is therefore important to understand more fully the basis for the apparent validity of the extended Abraham model and, even more important, to determine the limitations of this approach.

Of all the phase changes involving neat liquids, vaporization should provide the most sensitive test of the extent to which the parameters used in a LSER-type correlation can appropriately model the intermolecular interactions present in a neat liquid. Therefore we have undertaken a study of the extent to which vapor pressure values correlate with the empirical solute parameters of Abraham. The results reported here provide a useful method for estimating the vapor pressures of organic compounds from their structures. In addition, the results both lead to a better understanding of the limitations of using LSER methods to model the properties of pure substances and also point to some methods to improve such correlations.

## Results and Discussion

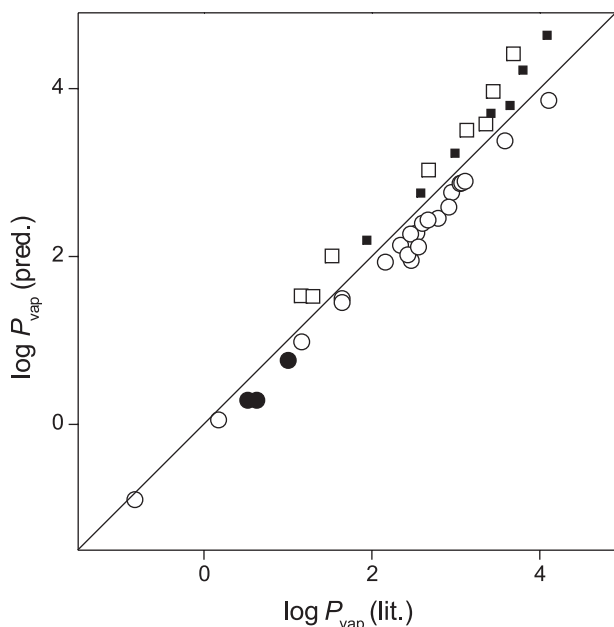
In order to avoid the complications of hydrogen bonding in the initial phase of the study, we considered first a group of 315 organic liquids having  $A$  values equal to or near 0. The data set included alkanes, cycloalkanes, alkenes, cycloalkenes, dienes, alkynes, benzene, alkylbenzenes, alkylnaphthalenes, alkyl halides, aryl halides, ethers, thioethers, aldehydes, ketones, esters, mercaptans, tertiary amines, pyridines, nitriles, and nitro compounds.<sup>14</sup> The resulting correlation of  $\log P_{\text{vap}}$  (in Pa, at 298 K) with the three non-specific solute parameters,  $V$ ,  $E$ , and  $S$ , is shown in equation 2.<sup>15,16</sup>

$$\log P_{\text{vap}} = 7.78 - 3.45 V - 0.93 E - 1.70 S \quad (2)$$

The fact that all of the coefficients in equation 2 are negative is chemically reasonable because all stabilizing intermolecular interactions decrease the vapor pressure of a liquid.<sup>9</sup> Additionally, equation 2 indicates that generalized dispersion is the dominant factor in determining the vapor pressure of compounds that do not hydrogen bond. That is, the effect of dispersion (given by the product  $3.45 V$ ) is greater than that of either of the other interactions ( $0.93 E$  or  $1.70 S$ ) for all of the compounds in the data set. In fact, the contribution of dispersion averages 77% of the total contribution of the  $V$ ,  $E$ , and  $S$  interactions for all of the compounds in the data set and is more than 50% for all but three compounds.<sup>17</sup>

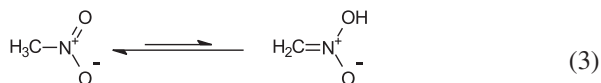
It is noteworthy that the correlation in equation 2 is so good because, as noted above, the solvent is different for each solute in the group. One might expect that the interactions of a solute molecule with identical solvent molecules would be similar for compounds that are close homologs, but the results suggest that such interactions are also similar among many different classes of compounds. In order to test that conclusion more fully, we checked for functional group-specific differences between literature values of  $\log P_{\text{vap}}$  and those predicted with equation 2. Such differences were indeed found for four families of compounds. The predicted values of  $\log P_{\text{vap}}$  were about 0.30 units too large for alkyl nitriles and about 0.41 units too large for alkyl nitro compounds. Alkylbenzenes as a group gave predicted values about 0.24 units too low, and predicted values for alkylnaphthalenes were about 0.27 units too small. These systematic deviations are illustrated in Figure 1.

It has been suggested<sup>18</sup> that deviation of a value for an aliphatic nitro compound predicted with an LSER may reflect some degree of tautomerization to the nitronic acid



**Figure 1.** Correlation of literature values of  $\log P_{\text{vap}}$  and those predicted with equation 2 for nitriles (■), nitro compounds (□), alkylbenzenes (○) and alkylnaphthalenes (●). The diagonal line represents a perfect correlation of literature and predicted values.

(as shown for nitromethane in equation 3), which could result in hydrogen-bonding interactions.<sup>19,20</sup>



The equilibrium constant for conversion of nitromethane to the nitronic acid in the gas phase is calculated to be  $2.2 \times 10^{-12}$ , however, and tautomerization of a nitronic acid to the isomeric alkane in the condensed phase is thought to be essentially complete.<sup>19</sup> Moreover, in aqueous solution and at cellular pH, aci-tautomerization of secondary nitroalkanes is much greater than that of primary nitroalkanes,<sup>21</sup> but the deviation between predicted and literature values of  $P_{\text{vap}}$  in the present study is much greater for 1-nitropropane than for 2-nitropropane. In addition, the average deviation between predicted and literature values of  $\log P_{\text{vap}}$  for a series of nitroalkanes is only slightly greater than the average deviation observed for nitrobenzene, *m*-nitrotoluene, and *o*-nitrotoluene.<sup>22</sup> Similarly, the average deviation between literature and predicted values for a set of alkyl nitriles is not much greater than that for nitrobenzene. Therefore hydrogen bonding arising from tautomerization seems not to explain our  $\log P_{\text{vap}}$  results.

Both cyano and nitro aliphatic compounds have significantly larger local dipole moments than do other compounds in the data set. This observation suggested that the lower than predicted vapor pressures of the nitriles

and nitro compounds might reflect an intrinsic limitation of the  $S$  parameter as a descriptor for the properties of neat liquids. Thus, if  $S$  reflects primarily the non-specific dipolar interactions of the solute with a surrounding dielectric medium, it will fail to account adequately for dipole-dipole interactions strong enough to cause some transient ordering of molecules in the liquid state.<sup>23</sup> An LSER correlation such as equation 2, which uses  $S$  as the only parameter for dipolar interaction, will therefore overestimate the vapor pressures of nitriles and nitro compounds, as we observed.

The situation is the opposite for nonpolar, aromatic compounds. There is strong correlation ( $R^2 = 0.97$ ) between the  $S$  and  $E$  values of those alkylbenzenes and alkylnaphthalenes in the data set. This correlation may lead to an overestimation of the stabilization due to dispersion interactions in the bulk liquid and consequently to an underestimation of the vapor pressure, as observed in Figure 1 for  $\log P_{\text{vap}}$  values predicted with equation 2.

The most direct way to compensate for the deviations noted above is to apply a functional group-specific adjustment ( $\lambda$ ) to the  $S$  parameter for these four classes of solutes. There is some precedent for this approach in the use of the “polarization correction” parameter  $\delta$  by Kamlet et al. to predict octanol/water partition coefficients.<sup>24</sup> Empirically, the best-fit values of  $\lambda$  were found to be +0.26 for aliphatic nitriles, +0.32 for nitro compounds, -0.20 for benzene and alkylbenzenes, and -0.32 for alkylnaphthalenes (with  $\lambda = 0$  for all other classes of compounds in the data set). For the former two, these  $\lambda$  values are qualitatively in line with the relative order of the magnitudes of the local dipole moments, and the  $\lambda$  values for the latter two follow the order of the polarizabilities of phenyl vs. naphthyl rings. The resulting correlation, given by equation 4, showed a substantial improvement in the  $F$  value and in the standard error of the prediction. Moreover, there was a substantial increase in the partial  $F$  values and a notable decrease in the standard errors of the coefficients of  $E$  and  $(S+\lambda)$  for the whole data set, again consistent with the proposed origin of the deviations for the four classes identified above.

$$\log P_{\text{vap}} = 7.86 - 3.54 V - 1.17 E - 1.52 (S + \lambda) \quad (4)$$

( $n = 315$ ,  $R^2 = 0.985$ ,  $F = 6930$ , standard error = 0.145)

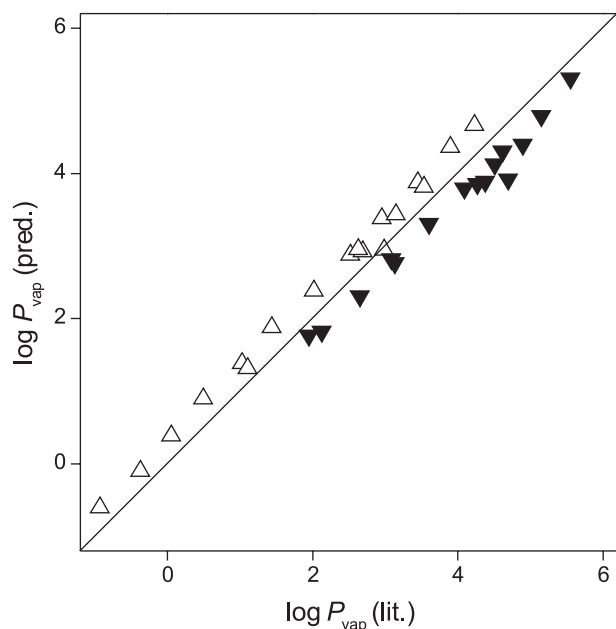
For compounds having values of both  $A$  and  $B$  significantly greater than 0, hydrogen bonding is expected to be the dominant type of specific interaction in the neat liquid. As in previous work,<sup>11,12</sup> we included the parameter  $A \times B$  to model the overall strength of hydrogen-bond interaction in the correlation (equation 5) for a data set of

376 compounds, which consisted of the original data set plus 61 alcohols, phenols, and amines.<sup>25</sup> The resulting correlation is shown in equation 5.

$$\log P_{\text{vap}} = 7.92 - 3.58 V - 1.15 E - 1.53 (S + \lambda) - 5.75 (A \times B) \quad (5)$$

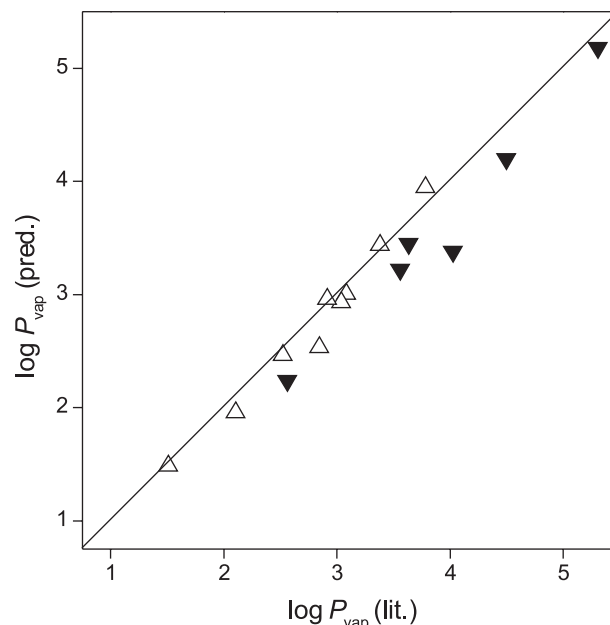
( $n = 376$ ,  $R^2 = 0.978$ ,  $F = 4088$ , standard error = 0.159)

Inspection of these results again revealed some interesting functional group-specific deviations between predicted and literature values. The predicted values of  $\log P_{\text{vap}}$  for primary alcohols were consistently about 0.37 units too large, while those for primary amines were about 0.37 units too small (Figure 2). Predicted values for secondary alcohols were close to the experimental values, while those for secondary amines were about 0.32 units too small (Figure 3).



**Figure 2.** Correlation of literature values of  $\log P_{\text{vap}}$  and those predicted with equation 5 for primary alcohols ( $\Delta$ ) and primary amines ( $\blacktriangledown$ ). The diagonal line represents a perfect correlation of literature and predicted values.

The simplest explanation for these discrepancies is that the product of the  $A$  and  $B$  values for a particular solute does not adequately quantify the hydrogen bonding interactions present in the neat liquid because of pronounced steric effects on self-association. Indeed, steric influences on hydrogen bonding have been reported previously for neat alcohols, phenols, and amines.<sup>26</sup> The most expedient way of correcting a LSER for steric effects on hydrogen bonding in neat liquids is by the inclusion of a scaling factor,  $\eta$ , as an empirical hydrogen-bonding index. Setting the value of  $\eta$  to 2.0 for primary alcohols resulted in best-fit values of  $\eta$  (to the nearest 0.01 unit) of 1.43 for secondary alcohols; 1.27 for tertiary alcohols, phenols,



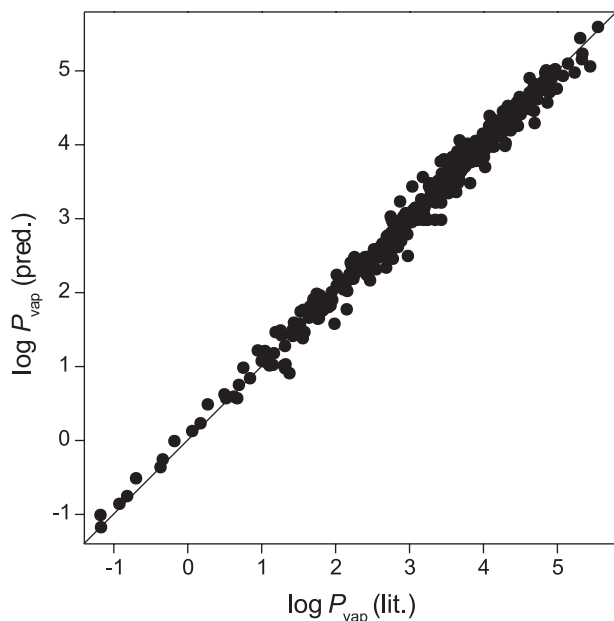
**Figure 3.** Correlation of literature values of  $\log P_{\text{vap}}$  and those predicted with equation 5 for secondary alcohols ( $\Delta$ ) and secondary amines ( $\blacktriangledown$ ). The diagonal line represents a perfect correlation of literature and predicted values.

and anilines; 0.61 for primary amines; and 0 for secondary amines. Such values of  $\eta$  for the alcohols are reminiscent of the 2.0 : 1.66 : 0.94 ratios reported for the relative self-association constants for 1-propanol, 2-propanol, and 2-methyl-2-propanol, respectively, in cyclohexane solution.<sup>26</sup> As with those equilibrium constants, the values of  $\eta$  reflect the decrease in net stabilization of clustered alcohol molecules as substitution around the hydroxyl group increases. Inclusion of the  $\eta$  parameter results in equation 6, which is a substantially better correlation than that in equation 5. In addition, the coefficients for the non-hydrogen bonding interaction terms in equation 6 are identical to those of equation 4, as would be expected if the separation of the hydrogen-bonding and non-hydrogen-bonding interactions described here is correct. The results for all 376 compounds are plotted in Figure 4.

$$\log P_{\text{vap}} = 7.86 - 3.54 V - 1.17 E - 1.52 (S + \lambda) - 3.64 (\eta \times A \times B) \quad (6)$$

( $n = 376$ ,  $R^2 = 0.986$ ,  $F = 6524$ , standard error = 0.148)

Equation 6 implicitly assumes that the attractive intermolecular interactions present in the neat liquid are lost when the liquid vaporizes. This assumption will not be true, and thus equation 6 will not apply, for two categories of compounds. The first includes compounds that are associated in the vapor phase, typically as a result of hydrogen bonding. For example, carboxylic acids have a strong tendency to dimerize in the neat liquid and – for the more volatile aliphatic



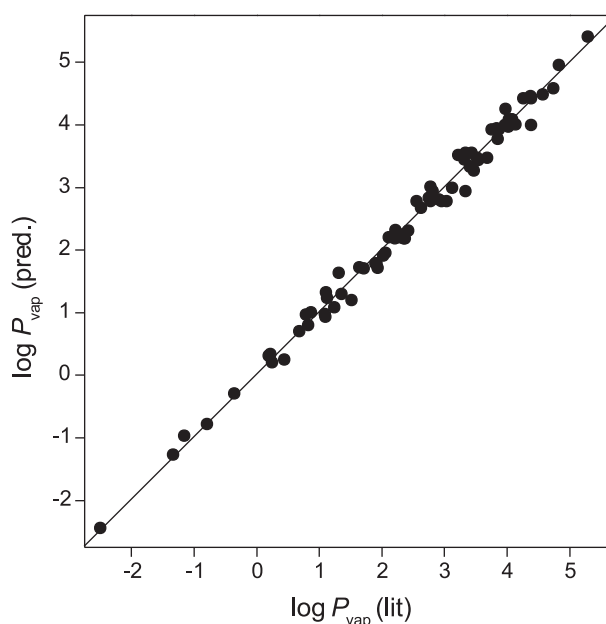
**Figure 4.** Correlation of values of predicted with equation 6 with literature  $\log P_{\text{vap}}$  values for all 376 compounds in the data set. The diagonal line represents a perfect correlation of literature and predicted values.

carboxylic acids – even in the vapor phase.<sup>27</sup> Since solute parameters are available only for monomeric carboxylic acids, values of  $\log P_{\text{vap}}$  predicted for carboxylic acids on the basis of equation 6 would exhibit poor agreement with literature values. The second category of compounds not well described by equation 6 includes compounds such as 2-alkoxyalcohols that exhibit some intramolecular hydrogen-bonding interactions as monomers in the gas phase.<sup>28</sup> In addition, highly polar compounds that show enhanced dipole-dipole attraction similar to that proposed for the nitriles and nitro compounds would require determination of an appropriate  $\lambda$  value before equation 6 could be applied to them.

Although equation 6 was derived by using solutes for which the appropriate parameters have been reported by Abraham, it can also be used to estimate vapor pressure from molecular structure. The  $V$  parameter can be calculated easily from the number of atoms, bonds, and rings in the molecule,<sup>8</sup> and a neural network method has been used to predict  $S$ .<sup>29</sup> Values of  $E$  can be calculated from the refractive index or computed from the molar refraction calculated at the sodium D line (578 nm).<sup>30</sup> In addition, several groups have reported multiparametric linear regression and neural network methods for the estimation of the  $E$ ,  $S$ ,  $A$ , and  $B$  parameters directly from molecular structure.<sup>31,32</sup>

An alternative approach for structures with a single functional group is to estimate the parameters for the compound from the parameters reported for analogous structures. We did that for an additional 76 compounds for

which literature values of  $\log P_{\text{vap}}$  are available but for which solute parameters had not been tabulated. The additional compounds included a cycloalkane, alkenes, alkynes, conjugated dienes, alkyl halides, alkylbenzenes, alkylnaphthalenes, sulfides, disulfides, ethers, aldehydes, ketones, mercaptans, amines, alcohols, and a phenol.<sup>33</sup> As shown in Figure 5, the correlation between predicted and literature values is comparable ( $R^2 = 0.990$ , standard error = 0.156) to that for compounds with known solute parameters. Thus the use of equation 6, along with readily accessible molecular solute parameters, offers a convenient way to estimate the vapor pressure of many organic liquids without recourse to experimentally determined values.



**Figure 5.** Correlation of values of  $\log P_{\text{vap}}$  predicted with equation 6 and solute parameters estimated from molecular structure with literature  $\log P_{\text{vap}}$  values for 76 additional compounds. The diagonal line represents a perfect correlation of literature and predicted values.

## Conclusions

The linear free solvation relationship method, which was developed to model the properties of a series of solutes in a given solvent system, can be extended to the prediction of physical properties of pure substances. However, it is necessary to demonstrate that the LSER applies equally well to all classes of compounds in the data set by looking for functional group-specific deviations from the overall correlation. Such deviations can be accommodated by the inclusion of additional parameters, but only if the chemical interpretation of such additional parameters is both clear and reasonable, as with the  $\eta$  and  $\lambda$  parameters developed here. This approach led to the development of equation 6,



which provides a convenient method for estimating the vapor pressure of pure organic liquids on the basis of solute parameters that can be found in the literature or deduced from molecular structure.

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## Supplementary Information

Empirical solute parameters and  $\log P_{\text{vap}}$  values for the compounds used to develop the LSER in equation 4, a table of empirical solute parameters estimated for specific functional groups, empirical solute parameters and  $\log P_{\text{vap}}$  values for the compounds used to develop the LSER shown in Figure 5, and partial  $F$  values for the parameters in equations 2 and 4. This material is available free of charge via the Internet at <http://jbc.sbcq.org.br>.

## References

1. Manahan, S. E.; *Fundamentals of Environmental Chemistry*, Lewis Publishers: Boca Raton, 1993.
2. Boethling, R. S.; Mackay, D.; *Handbook of Property Estimation Methods for Chemicals: Environmental and Health Sciences*, Lewis Publishers: Boca Raton, 2000.
3. For an introduction to and comparison of several methods, see Lyman, W. J.; Reehl, W. F.; Rosenblatt, D. H.; *Handbook of Chemical Property Estimation Methods*, McGraw-Hill: New York, 1982; Schwarzenbach, R. P.; Geschwend, P. M.; Imboden, D. M.; *Environmental Organic Chemistry*, 2<sup>nd</sup> ed., Wiley-Interscience: Hoboken, NJ, 2002, chapter 4. See also Mackay, D.; Bobra, A.; Chan, D. W.; Shiu, W.Y.; *Environ. Sci. Technol.* **1982**, *16*, 645.
4. See, for example, Katritzky, A. R.; Wang, Y.; Sild, S.; Tamm, T.; *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 720; McClelland, H. E.; Jurs, P. C.; *J. Chem. Inf. Comput. Sci.* **2000**, *40*, 967; Chalk, A. J.; Beck, B.; Clark, T.; *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 1053.
5. Kamlet, M. J.; Abboud, J. L. M.; Taft, R. W.; *Prog. Phys. Org. Chem.* **1981**, *13*, 485.
6. Abraham, M. H.; *Chem. Soc. Rev.* **1993**, 73.
7. Abraham, M. H.; Gola, J. M. R.; Cometto-Muniz, J. E.; Cain, W. S.; *J. Chem. Soc., Perkin Trans. 2* **2000**, 2067.
8. Abraham, M. H.; McGowan, J. C.; *Chromatographia* **1987**, *23*, 243. See also the note on p. 83 of reference 6 regarding the counting of rings and bonds in the structure.
9. Bel'skii, V. E.; *Russian Chem. Bull.* **2002**, *51*, 2008. (CA 138:169822). The physical significance of the  $V^2$  term was not discussed.
10. For examples and leading references, see reference 6; Abraham, M. H.; Martins, F.; *J. Pharm. Sci.* **2004**, *93*, 1508; Abraham, M. H.; *J. Environ. Monit.* **2003**, *5*, 747; Monarrez, C. I.; Acree, W. E., Jr.; Abraham, M. H.; *Phys. Chem. Liq.* **2002**, *40*, 581; Abraham, M. H.; Zissimos, A. M.; Acree, W. E., Jr.; *Phys. Chem. Chem. Phys.* **2001**, *3*, 3732.
11. Freitas, A. A.; Quina, F. H.; Carroll, F. A.; *J. Phys. Chem. B* **1997**, *101*, 7488.
12. Freitas, A. A.; Quina, F. H.; Carroll, F. A.; *Langmuir* **2000**, *16*, 6689.
13. Abraham, M. H.; Le, J.; *J. Pharm. Sci.* **1999**, *88*, 868.
14. Some haloalkanes had  $A$  values near 0.15, and terminal alkynes had  $A$  values near 0.12. Most other compounds had  $A$  values of 0, but a few had values around 0.05. A full listing of the compounds and their solute parameters is provided in the Supplementary Information.
15. Values of  $P_{\text{vap}}$  and molecular dipole moments were obtained from the DIPPR database (available from DIPPR 801 Project, 350 CB, Brigham Young University, Provo, UT 84602). Values of the Abraham parameters were obtained from Abraham, M. H.; Chadha, H. S.; Whiting, G. S.; Mitchell, R. C.; *J. Pharm. Sci.* **1994**, *83*, 1085 or from reference 6.
16. We also considered that the form of the correlation might be  $\log P_{\text{vap}} = c - vV^2 - eE^2 - sS^2$  but we found that replacing any of the three parameters in equation 2 with the square of that parameter made the resulting correlation worse instead of better.
17. Those three compounds are nitromethane, acetonitrile, and pyrimidine, and even for these compounds the contribution of dispersion is greater than 40% of the total contribution of the  $V$ ,  $E$ , and  $S$  terms for each substance.
18. Kamlet, M. J.; Doherty, R. M.; Abraham, M. H.; Marcus, Y.; Taft, R. W.; *J. Phys. Chem.* **1988**, *92*, 5244.
19. Nielsen, A. T. In *The Chemistry of the Nitro and Nitroso Groups*; Feuer, H., ed.; Interscience: New York, 1969, Part 1, p. 349.
20. Lammertsma, K.; Prasad, B. V.; *J. Am. Chem. Soc.* **1993**, *115*, 2348.
21. Löfroth, G.; Nilsson, L.; Andersen, J. R.; *Prog. Clin. Biol. Res.* **1986**, *209B*, 149.
22. The average deviation for nitroethane, 1-nitropropane, 2-nitropropane, and 1-nitrobutane was -0.37 log units, while that for nitrobenzene, *o*-nitrotoluene and *m*-nitrotoluene was -0.36 log units. The average deviation for propionitrile, butyronitrile, isobutyronitrile, valeronitrile, and hexanenitrile was -0.30 log units, while that for benzonitrile was -0.26 log units.

23. Huyskens, P. L.; *J. Mol. Struct.* **1989**, *198*, 123.
24. Kamlet *et al.*<sup>18</sup> included the term ( $\pi^* + d\delta$ ), where  $d$  is a function of the extent to which polarizability is a significant contributor to the property being modeled.
25. The additional compounds included 30 alcohols, 21 alkyl amines, 7 aryl amines and related compounds, and 3 phenols. The complete list of compounds is given in the Supplementary Information.
26. Frange, B.; Abboud, J.-L. M.; Benamou, C.; Bellon, L.; *J. Org. Chem.* **1982**, *47*, 4553. One possible reason that the ratios of the  $\eta$  values we used deviate slightly from the ratios of association constants is that the product ( $A \times B$ ) increases from 1-propanol to 2-propanol to 2-methyl-2-propanol.
27. Jaspersen, L. V.; Wilson, L. C.; Brady, C. J.; Wilding, W. V.; Wilson, G. M.; *AIChE Symposium Series* **1989**, *85*, 102; Curtiss, L.A.; Blander, M.; *Chem. Rev.* **1988**, *88*, 827.
28. See, for example, Yasuda, T.; Ikawa, S.; *J. Chem. Soc., Faraday Trans.* **1997**, *93*, 1869; Kowski, K.; Luttke, W.; Rademacher, P.; *J. Mol. Struct.* **2001**, *567-568*, 231.
29. Soil, D.; Ševčík, J. G. K.; Kvasnika, V.; *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 338.
30. Lima, G. A. R.; *PhD. Thesis*, Universidade de São Paulo, Brazil, 2000.
31. Platts, J. A.; Butina, D.; Abraham, M. H.; Hersey, A.; *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 835; Abraham, M. H.; Platts, J. A.; *J. Org. Chem.* **2001**, *66*, 3484; Jover, J.; Bosque, R.; Sales, J.; *J. Chem. Inf. Comput. Sci.* **2004**, *44*, 1098.
32. A referee has pointed out that the solute parameters can also be calculated with commercial software available from Pharma Algorithms.
33. The specific compounds, their estimated parameters, and the predicted and literature values of  $\log P_{\text{vap}}$  are given in the Supplementary Information.

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## A Linear Solvation Energy Relationship to Predict Vapor Pressure from Molecular Structure

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**Table S1.** Parameters and log  $P_{vap}$  values used to develop the LSER

No.	Compound	$P_{vap}$ (Pa)	Source	Error	Predicted		A	B	V	E	S	$\lambda$	$\eta$
					log $P_{vap}$	log $P_{vap}$							
1	n-pentane	6.84E+04	E	<3%	4.835	4.984	0	0	0.813	0	0	0	0
2	isopentane	9.17E+04	EP	<3%	4.962	4.984	0	0	0.813	0	0	0	0
3	n-hexane	2.03E+04	E	<3%	4.307	4.484	0	0	0.954	0	0	0	0
4	3-methylpentane	2.52E+04	E	<3%	4.402	4.484	0	0	0.954	0	0	0	0
5	n-heptane	6.07E+03	E	<3%	3.783	3.984	0	0	1.095	0	0	0	0
6	n-octane	1.87E+03	E	<3%	3.272	3.485	0	0	1.236	0	0	0	0
7	n-nonane	5.80E+02	E	<3%	2.764	2.986	0	0	1.377	0	0	0	0
8	n-decane	1.81E+02	E	<3%	2.258	2.486	0	0	1.518	0	0	0	0
9	n-undecane	5.56E+01	E	<3%	1.745	1.985	0	0	1.659	0	0	0	0
10	n-dodecane	1.79E+01	E	<3%	1.252	1.489	0	0	1.799	0	0	0	0
11	n-tridecane	5.69E+00	E	<1%	0.755	0.988	0	0	1.940	0	0	0	0
12	n-tetradecane	1.86E+00	E	<3%	0.270	0.489	0	0	2.081	0	0	0	0
13	n-pentadecane	6.55E-01	E	<3%	-0.184	-0.011	0	0	2.222	0	0	0	0
14	n-hexadecane	1.99E-01	E	<3%	-0.700	-0.510	0	0	2.363	0	0	0	0
15	n-heptadecane	6.62E-02	E	<5%	-1.179	-1.009	0	0	2.504	0	0	0	0
16	4-methylnonane	3.09E+02	EP	<3%	2.490	2.486	0	0	1.518	0	0	0	0
17	2-methyloctane	8.44E+02	E	<3%	2.927	2.986	0	0	1.377	0	0	0	0
18	3-methyloctane	8.33E+02	EP	<3%	2.921	2.986	0	0	1.377	0	0	0	0
19	2-methylpentane	2.81E+04	E	<3%	4.449	4.484	0	0	0.954	0	0	0	0
20	2-methylhexane	8.77E+03	E	<3%	3.943	3.984	0	0	1.095	0	0	0	0
21	3-methylhexane	8.19E+03	E	<3%	3.913	3.984	0	0	1.095	0	0	0	0
22	2-methylheptane	2.75E+03	E	<3%	3.439	3.485	0	0	1.236	0	0	0	0
23	3-methylheptane	2.61E+03	E	<3%	3.417	3.485	0	0	1.236	0	0	0	0
24	4-methylheptane	2.73E+03	E	<3%	3.436	3.485	0	0	1.236	0	0	0	0
25	3-ethylhexane	2.68E+03	E	<3%	3.428	3.485	0	0	1.236	0	0	0	0
26	3-methylnonane	2.64E+02	EP	<3%	2.421	2.486	0	0	1.518	0	0	0	0
27	2-methylnonane	2.51E+02	EP	<3%	2.400	2.486	0	0	1.518	0	0	0	0
28	5-methylnonane	2.94E+02	EP	<3%	2.468	2.486	0	0	1.518	0	0	0	0
29	4-methyloctane	9.10E+02	EP	<3%	2.959	2.986	0	0	1.377	0	0	0	0
30	3-methylundecane	2.57E+01	EP	<10%	1.411	1.489	0	0	1.799	0	0	0	0
31	neopentane	1.71E+05	E	<1%	5.234	4.984	0	0	0.813	0	0	0	0
32	2,2-dimethylbutane	4.27E+04	E	<3%	4.631	4.484	0	0	0.954	0	0	0	0
33	2,3-dimethylbutane	3.13E+04	E	<3%	4.496	4.484	0	0	0.954	0	0	0	0
34	2,2-dimethylpentane	1.40E+04	E	<3%	4.147	3.984	0	0	1.095	0	0	0	0
35	2,3-dimethylpentane	9.17E+03	E	<3%	3.962	3.984	0	0	1.095	0	0	0	0
36	2,4-dimethylpentane	1.31E+04	E	<3%	4.118	3.984	0	0	1.095	0	0	0	0
37	3,3-dimethylpentane	1.10E+04	E	<3%	4.042	3.984	0	0	1.095	0	0	0	0
38	2,2-dimethylhexane	4.54E+03	E	<3%	3.657	3.485	0	0	1.236	0	0	0	0
39	2,3-dimethylhexane	3.13E+03	E	<3%	3.495	3.485	0	0	1.236	0	0	0	0
40	2,4-dimethylhexane	4.05E+03	E	<1%	3.607	3.485	0	0	1.236	0	0	0	0
41	2,5-dimethylhexane	4.04E+03	E	<3%	3.606	3.485	0	0	1.236	0	0	0	0
42	3,3-dimethylhexane	3.81E+03	E	<3%	3.581	3.485	0	0	1.236	0	0	0	0

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Table S1. (cont.)

No.	Compound	$P_{\text{vap}}$ (Pa)	Source	Error	Predicted								
					$\log P_{\text{vap}}$	$\log P_{\text{vap}}$	$A$	$B$	$V$	$E$	$S$	$\lambda$	$\eta$
43	3,4-dimethylhexane	2.89E+03	E	<1%	3.461	3.485	0	0	1.236	0	0	0	0
44	2,2-dimethyloctane	4.85E+02	E	<3%	2.686	2.486	0	0	1.518	0	0	0	0
45	2,2-dimethylheptane	1.53E+03	EP	<5%	3.183	2.986	0	0	1.377	0	0	0	0
46	2,4,4-trimethylhexane	1.79E+03	EP	<5%	3.253	2.986	0	0	1.377	0	0	0	0
47	3-ethylpentane	7.75E+03	E	<3%	3.890	3.984	0	0	1.095	0	0	0	0
48	2,2,3-trimethylbutane	1.37E+04	E	<3%	4.135	3.984	0	0	1.095	0	0	0	0
49	2-methyl-3-ethylpentane	3.19E+03	E	<3%	3.503	3.485	0	0	1.236	0	0	0	0
50	3-methyl-3-ethylpentane	3.06E+03	E	<3%	3.486	3.485	0	0	1.236	0	0	0	0
51	2,2,3-trimethylpentane	4.28E+03	E	<1%	3.631	3.485	0	0	1.236	0	0	0	0
52	2,2,4-trimethylpentane	6.58E+03	E	<3%	3.818	3.485	0	0	1.236	0	0	0	0
53	2,3,3-trimethylpentane	3.60E+03	E	<3%	3.556	3.485	0	0	1.236	0	0	0	0
54	2,3,4-trimethylpentane	3.62E+03	E	<3%	3.558	3.485	0	0	1.236	0	0	0	0
55	2,2,5-trimethylhexane	2.22E+03	E	<3%	3.347	2.986	0	0	1.377	0	0	0	0
56	3,3,5-trimethylheptane	5.57E+02	EP	<3%	2.746	2.486	0	0	1.518	0	0	0	0
57	3,3-diethylpentane	9.72E+02	EP	<3%	2.988	2.986	0	0	1.377	0	0	0	0
58	2,2,3,3-tetramethylpentane	1.27E+03	E	<3%	3.103	2.986	0	0	1.377	0	0	0	0
59	2,2,3,4-tetramethylpentane	1.69E+03	EP	<5%	3.228	2.986	0	0	1.377	0	0	0	0
60	2,2,4,4-tetramethylpentane	2.67E+03	E	<3%	3.427	2.986	0	0	1.377	0	0	0	0
61	2,3,3,4-tetramethylpentane	1.18E+03	E	<5%	3.073	2.986	0	0	1.377	0	0	0	0
62	2,2,3,3-tetramethylhexane	1.81E+02	E	<3%	2.258	2.486	0	0	1.518	0	0	0	0
63	2,2,5,5-tetramethylhexane	5.37E+02	EP	<3%	2.730	2.486	0	0	1.518	0	0	0	0
64	3-ethylheptane	9.03E+02	P	<5%	2.956	2.986	0	0	1.377	0	0	0	0
65	cyclopentane	4.23E+04	E	<3%	4.627	4.908	0	0	0.705	0.263	0.100	0	0
66	cyclohexane	1.30E+04	E	<1%	4.115	4.363	0	0	0.845	0.305	0.100	0	0
67	cis-decalin	1.05E+02	E	<5%	2.019	2.242	0	0	1.300	0.544	0.250	0	0
68	trans-decalin	1.65E+02	E	<5%	2.218	2.362	0	0	1.300	0.467	0.230	0	0
69	cycloheptane	2.91E+03	E	<3%	3.464	3.809	0	0	0.986	0.35	0.100	0	0
70	cyclooctane	7.52E+02	E	<3%	2.876	3.237	0	0	1.127	0.413	0.100	0	0
71	methylcyclopentane	1.83E+04	E	<3%	4.263	4.456	0	0	0.845	0.225	0.100	0	0
72	methylcyclohexane	6.14E+03	E	<3%	3.788	3.934	0	0	0.986	0.244	0.100	0	0
73	cis-1,2-dimethylcyclohexane	1.93E+03	E	<3%	3.286	3.391	0	0	1.127	0.281	0.100	0	0
74	trans-1,2-dimethylcyclohexane	2.58E+03	E	<3%	3.412	3.496	0	0	1.127	0.191	0.100	0	0
75	1-pentene	8.51E+04	E	<3%	4.930	4.906	0	0.07	0.770	0.093	0.080	0	0
76	2-methyl-1-butene	8.13E+04	EP	<3%	4.910	4.941	0	0.07	0.770	0.063	0.080	0	0
77	2-methyl-2-butene	6.25E+04	E	<3%	4.796	4.829	0	0.07	0.770	0.159	0.080	0	0
78	1-hexene	2.47E+04	E	<3%	4.392	4.424	0	0.07	0.911	0.078	0.080	0	0
79	2-methyl-1-pentene	2.61E+04	E	<3%	4.416	4.410	0	0.07	0.911	0.09	0.080	0	0
80	1-heptene	7.51E+03	E	<3%	3.876	3.908	0	0.07	1.052	0.092	0.080	0	0
81	1-octene	2.33E+03	E	<3%	3.367	3.405	0	0.07	1.193	0.094	0.080	0	0
82	1-nonene	7.20E+02	E	<3%	2.857	2.910	0	0.07	1.334	0.09	0.080	0	0
83	1-decene	2.27E+02	E	<3%	2.355	2.409	0	0.07	1.475	0.093	0.080	0	0
84	1-undecene	6.71E+01	E	<3%	1.827	1.911	0	0.07	1.616	0.091	0.080	0	0
85	1-dodecene	2.65E+01	E	<3%	1.423	1.414	0	0.07	1.756	0.089	0.080	0	0
86	cyclohexene	1.19E+04	E	<3%	4.076	4.258	0	0.1	0.802	0.395	0.200	0	0
87	indene	1.45E+02	E	<5%	2.161	2.025	0	0.2	0.988	1.001	0.770	0	0
88	cis-2-pentene	6.60E+04	E	<1%	4.820	4.850	0	0.07	0.770	0.141	0.080	0	0
89	3-methyl-1-butene	1.20E+05	E	<3%	5.080	4.941	0	0.07	0.770	0.063	0.080	0	0
90	cyclopentene	5.04E+04	E	<3%	4.703	4.826	0	0.1	0.662	0.335	0.200	0	0
91	cycloheptene	3.34E+03	E	<3%	3.524	3.705	0	0.1	0.943	0.414	0.220	0	0
92	1-methylcyclopentene	1.55E+04	EP	<10%	4.190	4.332	0	0.1	0.802	0.33	0.200	0	0
93	1,3-butadiene	2.81E+05	E	<1%	5.449	5.065	0	0.1	0.586	0.32	0.230	0	0
94	1,4-pentadiene	9.80E+04	EP	<3%	4.991	4.768	0	0.1	0.727	0.185	0.200	0	0
95	2-methyl-1,3-butadiene	7.34E+04	E	<3%	4.866	4.574	0	0.1	0.727	0.313	0.230	0	0
96	1,5-hexadiene	2.96E+04	EP	<5%	4.471	4.262	0	0.1	0.868	0.191	0.200	0	0
97	1,4-hexadiene	2.33E+04	E	<3%	4.367	4.203	0	0.1	0.868	0.241	0.200	0	0
98	2,3-dimethyl-1,3-butadiene	2.02E+04	E	<3%	4.305	4.028	0	0.14	0.868	0.352	0.230	0	0
99	1,3-cyclohexadiene	1.30E+04	E	<3%	4.113	4.118	0	0.14	0.759	0.515	0.300	0	0
100	1,4-cyclohexadiene	8.72E+03	EP	<10%	3.940	4.058	0	0.17	0.759	0.501	0.350	0	0
101	1,5-cyclooctadiene	6.59E+02	EP	<5%	2.819	2.925	0	0.2	1.041	0.603	0.360	0	0
102	carbon tetrachloride	1.52E+04	E	<1%	4.182	4.134	0	0	0.739	0.458	0.380	0	0
103	1,4-dichlorobutane	5.08E+02	EP	<10%	2.706	2.687	0	0.17	0.917	0.413	0.950	0	0
104	dichloromethane	5.84E+04	E	<3%	4.766	4.795	0.1	0.05	0.494	0.387	0.570	0	0

Table S1. (cont.)

No.	Compound	$P_{\text{vap}}$ (Pa)	Source	Error	Predicted								
					$\log P_{\text{vap}}$	$\log P_{\text{vap}}$	$A$	$B$	$V$	$E$	$S$	$\lambda$	$\eta$
105	chloroform	2.62E+04	E	<3%	4.418	4.437	0.15	0.02	0.617	0.425	0.490	0	0
106	1,1-dichloroethane	3.03E+04	E	<3%	4.481	4.493	0.1	0.1	0.635	0.322	0.490	0	0
107	1,2-dichloroethane	1.06E+04	E	<1%	4.027	4.155	0.1	0.11	0.635	0.416	0.640	0	0
108	1,1,2-trichloroethane	3.09E+03	EP	<3%	3.489	3.565	0.13	0.13	0.757	0.499	0.680	0	0
109	1,2-dichloropropane	6.89E+03	EP	<3%	3.838	3.769	0.1	0.11	0.776	0.371	0.600	0	0
110	1,1,1-trichloroethane	1.66E+04	E	<5%	4.221	4.128	0	0.09	0.757	0.369	0.410	0	0
111	1,1,1,2-tetrachloroethane	1.60E+03	E	<3%	3.205	3.155	0.1	0.08	0.880	0.542	0.630	0	0
112	1,1,2,2-tetrachloroethane	7.65E+02	E	<5%	2.884	2.896	0.16	0.12	0.880	0.595	0.760	0	0
113	isopropyl chloride	6.87E+04	EP	<5%	4.837	4.808	0	0.12	0.654	0.177	0.350	0	0
114	isobutyl chloride	2.00E+04	E	<5%	4.301	4.261	0	0.12	0.795	0.191	0.370	0	0
115	2-chloro-2-methylpropane	4.09E+04	EP	<5%	4.612	4.501	0	0.12	0.795	0.142	0.250	0	0
116	trichloroethylene	9.83E+03	E	<3%	3.992	4.157	0.08	0.03	0.715	0.524	0.370	0	0
117	tetrachloroethylene	2.47E+03	E	<3%	3.393	3.484	0	0	0.837	0.639	0.440	0	0
118	allyl chloride	4.88E+04	EP	<5%	4.688	4.466	0	0.05	0.611	0.327	0.560	0	0
119	cis-1,2-dichloroethene	2.72E+04	E	<3%	4.435	4.329	0.11	0.05	0.592	0.436	0.610	0	0
120	trans-1,2-dichloroethene	4.45E+04	E	<5%	4.648	4.647	0.09	0.05	0.592	0.425	0.410	0	0
121	n-propyl chloride	4.59E+04	E	<3%	4.662	4.686	0	0.1	0.654	0.216	0.400	0	0
122	n-butyl chloride	1.35E+04	E	<3%	4.131	4.194	0	0.1	0.795	0.21	0.400	0	0
123	sec-butyl chloride	2.09E+04	E	<3%	4.321	4.294	0	0.12	0.795	0.189	0.350	0	0
124	1-chloropentane	4.36E+03	E	<3%	3.640	3.696	0	0.1	0.936	0.208	0.400	0	0
125	pentachloroethane	4.89E+02	E	<5%	2.690	2.554	0.17	0.06	1.002	0.648	0.660	0	0
126	1,1-dichloroethene	7.99E+04	E	<5%	4.903	4.827	0	0.05	0.592	0.362	0.340	0	0
127	ethyl iodide	1.80E+04	E	<3%	4.254	4.210	0	0.15	0.649	0.64	0.400	0	0
128	n-propyl iodide	5.74E+03	E	<3%	3.759	3.718	0	0.15	0.790	0.634	0.400	0	0
129	tribromomethane	7.34E+02	EP	<5%	2.866	2.948	0.15	0.06	0.775	0.974	0.680	0	0
130	1,3-dichloropropane	2.43E+03	EP	<5%	3.386	3.513	0	0.17	0.776	0.408	0.740	0	0
131	halothane	4.01E+04	E	<5%	4.603	4.541	0.15	0.05	0.741	0.102	0.380	0	0
132	methyl bromide	2.18E+05	E	<3%	5.339	5.239	0	0.1	0.425	0.399	0.430	0	0
133	bromoethane	6.30E+04	E	<3%	4.799	4.827	0	0.12	0.565	0.366	0.400	0	0
134	1-bromopropane	1.84E+04	E	<3%	4.266	4.327	0	0.12	0.706	0.366	0.400	0	0
135	2-bromopropane	2.89E+04	E	<3%	4.460	4.443	0	0.14	0.706	0.332	0.350	0	0
136	1-bromobutane	5.59E+03	E	<5%	3.748	3.835	0	0.12	0.847	0.36	0.400	0	0
137	1-bromoheptane	1.70E+02	E	<3%	2.229	2.355	0	0.12	1.270	0.343	0.400	0	0
138	methyl iodide	5.40E+04	E	<3%	4.732	4.622	0	0.13	0.508	0.676	0.430	0	0
139	dibromomethane	6.03E+03	EP	<3%	3.780	3.888	0.1	0.1	0.600	0.714	0.670	0	0
140	diiodomethane	1.60E+02	E	<5%	2.205	2.407	0.05	0.23	0.766	1.453	0.690	0	0
141	1-iodohexane	1.53E+02	EP	<10%	2.185	2.243	0	0.15	1.212	0.615	0.400	0	0
142	1-iodobutane	1.81E+03	E	<3%	3.258	3.227	0	0.15	0.930	0.628	0.400	0	0
143	benzyl chloride	1.74E+02	P	<3%	2.240	2.187	0	0.33	0.980	0.821	0.820	0	0
144	chlorobenzene	1.59E+03	EP	<5%	3.200	3.065	0	0.07	0.839	0.718	0.650	0	0
145	o-dichlorobenzene	1.81E+02	E	<3%	2.257	2.256	0	0.04	0.961	0.872	0.780	0	0
146	m-dichlorobenzene	2.86E+02	E	<3%	2.457	2.361	0	0.02	0.961	0.847	0.730	0	0
147	o-chlorotoluene	4.70E+02	EP	<3%	2.672	2.514	0	0.07	0.980	0.762	0.650	0	0
148	p-chlorotoluene	3.72E+02	EP	<5%	2.570	2.550	0	0.07	0.980	0.705	0.670	0	0
149	1,2,4-trichlorobenzene	5.74E+01	E	<3%	1.759	1.648	0	0	1.084	0.98	0.810	0	0
150	m-dibromobenzene	3.58E+01	EP	<10%	1.554	1.384	0	0.04	1.066	1.17	0.880	0	0
151	bromobenzene	5.68E+02	E	<3%	2.754	2.568	0	0.09	0.891	0.882	0.730	0	0
152	fluorobenzene	1.03E+04	E	<3%	4.012	3.840	0	0.1	0.734	0.477	0.570	0	0
153	benzotrifluoride	4.97E+03	E	<5%	3.696	3.647	0	0.1	0.910	0.225	0.480	0	0
154	iodobenzene	1.42E+02	E	<3%	2.151	1.777	0	0.12	0.975	1.188	0.820	0	0
155	methyl ethyl sulfide	2.13E+04	E	<3%	4.329	4.369	0	0.28	0.695	0.39	0.380	0	0
156	di-n-propyl sulfide	8.89E+02	E	<3%	2.949	2.907	0	0.32	1.118	0.358	0.380	0	0
157	diethyl sulfide	8.02E+03	E	<3%	3.904	3.889	0	0.32	0.836	0.373	0.380	0	0
158	dimethyl sulfide	6.46E+04	E	<3%	4.810	4.853	0	0.29	0.554	0.404	0.380	0	0
159	thiophene	1.05E+04	E	<3%	4.022	3.940	0	0.15	0.641	0.687	0.560	0	0
160	diethyl disulfide	5.67E+02	EP	<3%	2.754	2.813	0	0.28	0.999	0.67	0.480	0	0
161	dimethyl disulfide	3.83E+03	E	<3%	3.583	3.843	0	0.28	0.717	0.695	0.440	0	0
162	carbon disulfide	4.78E+04	E	<1%	4.680	4.785	0	0.07	0.491	0.877	0.210	0	0
163	2-methylthiophene	3.30E+03	E	<3%	3.519	3.439	0	0.16	0.782	0.688	0.560	0	0
164	paraldehyde	1.46E+03	EP	<5%	3.164	3.049	0	0.68	1.022	0.136	0.680	0	0
165	diethylether	7.17E+04	E	<3%	4.856	4.846	0	0.45	0.731	0.041	0.250	0	0
166	diisopropyl ether	1.98E+04	E	<3%	4.297	3.986	0	0.41	1.013	0	0.190	0	0

Table S1. (cont.)

No.	Compound	$P_{\text{vap}}$ (Pa)	Source	Error	Predicted								
					$\log P_{\text{vap}}$	$\log P_{\text{vap}}$	$A$	$B$	$V$	$E$	$S$	$\lambda$	$\eta$
167	di-n-butyl ether	8.37E+02	EP	<5%	2.923	2.896	0	0.45	1.295	0	0.250	0	0
168	methyl n-propyl ether	6.10E+04	E	<5%	4.785	4.824	0	0.45	0.731	0.06	0.250	0	0
169	di-n-propyl ether	8.30E+03	E	<5%	3.919	3.801	0	0.45	1.013	0.08	0.250	0	0
170	anisole	4.83E+02	E	<3%	2.684	2.652	0	0.29	0.916	0.708	0.750	0	0
171	1,4-dioxane	5.09E+03	E	<1%	3.707	3.926	0	0.64	0.681	0.329	0.750	0	0
172	1,2-propylene oxide	7.13E+04	E	<5%	4.853	5.009	0	0.45	0.481	0.243	0.570	0	0
173	furan	8.00E+04	E	<3%	4.903	4.728	0	0.13	0.536	0.369	0.530	0	0
174	tetrahydrofuran	2.15E+04	E	<1%	4.333	4.532	0	0.48	0.622	0.289	0.520	0	0
175	propanal	4.25E+04	E	<3%	4.628	4.708	0	0.45	0.547	0.196	0.650	0	0
176	butanal	1.50E+04	E	<3%	4.175	4.219	0	0.45	0.688	0.187	0.650	0	0
177	2-methylpropanal	2.11E+04	EP	<3%	4.324	4.315	0	0.45	0.688	0.144	0.620	0	0
178	pentanal	4.58E+03	E	<5%	3.661	3.747	0	0.45	0.829	0.163	0.650	0	0
179	heptanal	5.12E+02	E	<5%	2.710	2.774	0	0.45	1.111	0.14	0.650	0	0
180	hexanal	1.45E+03	E	<5%	3.162	3.267	0	0.45	0.970	0.146	0.650	0	0
181	octanal	1.54E+02	E	<10%	2.187	2.251	0	0.45	1.252	0.16	0.650	0	0
182	nonanal	3.66E+01	E	<5%	1.564	1.767	0	0.45	1.392	0.15	0.650	0	0
183	trans-crotonaldehyde	4.42E+03	EP	<5%	3.645	3.910	0	0.5	0.645	0.387	0.800	0	0
184	o-tolualdehyde	6.34E+01	EP	<25%	1.802	1.796	0	0.4	1.014	0.87	0.960	0	0
185	p-tolualdehyde	3.38E+01	P	<5%	1.529	1.744	0	0.42	1.014	0.862	1.000	0	0
186	benzaldehyde	1.70E+02	E	<5%	2.229	2.293	0	0.39	0.873	0.82	1.000	0	0
187	m-tolualdehyde	4.50E+01	EP	<10%	1.653	1.816	0	0.42	1.014	0.84	0.970	0	0
188	acetone	3.08E+04	E	<3%	4.488	4.652	0.04	0.49	0.547	0.179	0.700	0	0
189	2-butanone	1.23E+04	E	<3%	4.090	4.167	0	0.51	0.688	0.166	0.700	0	0
190	3-pentanone	4.97E+03	E	<3%	3.697	3.742	0	0.51	0.829	0.154	0.660	0	0
191	methyl isobutyl ketone	2.65E+03	E	<10%	3.423	3.308	0	0.51	0.970	0.111	0.650	0	0
192	4-heptanone	7.71E+02	EP	<10%	2.887	2.791	0	0.51	1.111	0.113	0.660	0	0
193	3-hexanone	1.85E+03	E	<3%	3.268	3.264	0	0.51	0.970	0.136	0.660	0	0
194	2-pentanone	4.74E+03	E	<3%	3.676	3.725	0	0.51	0.829	0.143	0.680	0	0
195	methyl isopropyl ketone	2.65E+03	E	<10%	3.423	3.781	0	0.51	0.829	0.134	0.650	0	0
196	2-hexanone	1.55E+03	E	<3%	3.191	3.233	0	0.51	0.970	0.136	0.680	0	0
197	2-heptanone	5.21E+02	E	<3%	2.717	2.749	0	0.51	1.111	0.123	0.680	0	0
198	5-methyl-2-hexanone	6.93E+02	EP	<3%	2.841	2.805	0	0.51	1.111	0.114	0.650	0	0
199	3,3-dimethyl-2-butanone	4.27E+03	E	<10%	3.630	3.361	0	0.51	0.970	0.106	0.620	0	0
200	5-nonanone	7.93E+01	E	<5%	1.899	1.806	0	0.51	1.392	0.103	0.660	0	0
201	2-nonanone	6.70E+01	EP	<5%	1.826	1.757	0	0.51	1.392	0.119	0.680	0	0
202	cyclopentanone	1.51E+03	E	<5%	3.178	3.569	0	0.52	0.720	0.373	0.860	0	0
203	cyclohexanone	5.52E+02	E	<3%	2.742	3.034	0	0.56	0.861	0.403	0.860	0	0
204	2-octanone	1.87E+02	EP	<10%	2.272	2.266	0	0.51	1.252	0.108	0.680	0	0
205	acetophenone	5.28E+01	E	<3%	1.722	1.780	0	0.48	1.014	0.818	1.010	0	0
206	methyl formate	7.80E+04	E	<1%	4.892	4.958	0	0.38	0.465	0.192	0.680	0	0
207	ethyl formate	3.26E+04	E	<1%	4.513	4.542	0	0.38	0.606	0.146	0.660	0	0
208	n-propyl formate	1.10E+04	E	<3%	4.041	4.104	0	0.38	0.747	0.132	0.630	0	0
209	n-butyl formate	3.85E+03	EP	<3%	3.585	3.619	0	0.38	0.888	0.121	0.630	0	0
210	isobutyl formate	5.47E+03	E	<3%	3.738	3.693	0	0.4	0.888	0.095	0.600	0	0
211	n-pentyl formate	1.19E+03	E	<5%	3.076	3.143	0	0.38	1.028	0.101	0.630	0	0
212	methyl propionate	1.14E+04	E	<1%	4.055	4.155	0	0.45	0.747	0.128	0.600	0	0
213	ethyl propionate	4.89E+03	E	<1%	3.690	3.733	0	0.45	0.888	0.087	0.580	0	0
214	n-propyl propionate	1.86E+03	E	<3%	3.270	3.287	0	0.45	1.028	0.07	0.560	0	0
215	n-propyl butanoate	7.77E+02	E	<5%	2.890	2.811	0	0.45	1.169	0.05	0.560	0	0
216	methyl butanoate	4.29E+03	E	<3%	3.633	3.681	0	0.45	0.888	0.106	0.600	0	0
217	ethyl butanoate	2.23E+03	E	<3%	3.349	3.259	0	0.45	1.028	0.068	0.580	0	0
218	methyl acrylate	1.16E+04	E	<3%	4.065	4.069	0	0.42	0.704	0.254	0.660	0	0
219	ethyl acrylate	5.00E+03	E	<5%	3.699	3.649	0	0.42	0.845	0.212	0.640	0	0
220	n-butyl acrylate	7.27E+02	E	<3%	2.861	2.724	0	0.42	1.126	0.177	0.620	0	0
221	methyl methacrylate	4.96E+03	E	<5%	3.695	3.641	0	0.45	0.845	0.245	0.620	0	0
222	ethyl methacrylate	2.71E+03	EP	<3%	3.433	3.224	0	0.45	0.986	0.2	0.600	0	0
223	isobutyl isobutyrate	5.95E+02	EP	<5%	2.775	2.461	0	0.47	1.310	0	0.500	0	0
224	isobutyl methacrylate	4.84E+02	EP	<5%	2.685	2.336	0	0.45	1.268	0.143	0.570	0	0
225	n-butyl methacrylate	2.77E+02	E	<10%	2.442	2.258	0	0.45	1.268	0.171	0.600	0	0
226	methyl decanoate	4.95E+00	EP	<10%	0.694	0.747	0	0.45	1.733	0.053	0.600	0	0
227	ethyl isobutyrate	3.38E+03	E	<3%	3.529	3.344	0	0.47	1.028	0.034	0.550	0	0
228	isobutyl acrylate	9.42E+02	E	<10%	2.974	2.794	0	0.42	1.126	0.156	0.590	0	0

Table S1. (cont.)

No.	Compound	$P_{\text{vap}}$ (Pa)	Source	Error	Predicted								
					$\log P_{\text{vap}}$	$\log P_{\text{vap}}$	$A$	$B$	$V$	$E$	$S$	$\lambda$	$\eta$
229	methyl acetate	2.86E+04	E	<1%	4.456	4.577	0	0.45	0.606	0.142	0.640	0	0
230	ethyl acetate	1.24E+04	E	<1%	4.094	4.150	0	0.45	0.747	0.106	0.620	0	0
231	n-propyl acetate	4.46E+03	E	<3%	3.649	3.697	0	0.45	0.888	0.092	0.600	0	0
232	n-butyl acetate	1.49E+03	E	<3%	3.174	3.225	0	0.45	1.028	0.071	0.600	0	0
233	isobutyl acetate	2.38E+03	E	<3%	3.376	3.293	0	0.47	1.028	0.052	0.570	0	0
234	isopentyl acetate	8.14E+02	E	<5%	2.910	2.794	0	0.47	1.169	0.051	0.570	0	0
235	allyl acetate	4.69E+03	EP	<5%	3.671	3.542	0	0.49	0.845	0.199	0.720	0	0
236	isopropyl acetate	8.05E+03	E	<3%	3.906	3.786	0	0.47	0.888	0.055	0.570	0	0
237	vinyl acetate	1.51E+04	EP	<5%	4.179	4.136	0	0.43	0.704	0.223	0.640	0	0
238	n-pentyl acetate	5.63E+02	EP	<5%	2.751	2.729	0	0.45	1.169	0.067	0.600	0	0
239	benzyl acetate	2.11E+01	EP	<10%	1.323	1.029	0	0.65	1.214	0.789	1.060	0	0
240	n-hexyl acetate	1.76E+02	E	<5%	2.244	2.243	0	0.45	1.310	0.056	0.600	0	0
241	n-heptyl acetate	5.79E+01	E	<5%	1.762	1.750	0	0.45	1.451	0.05	0.600	0	0
242	n-octyl acetate	2.07E+01	EP	<10%	1.316	1.275	0	0.45	1.592	0.029	0.600	0	0
243	n-butyl benzoate	4.67E+00	E	<10%	0.670	0.570	0	0.46	1.495	0.668	0.800	0	0
244	methyl benzoate	5.03E+01	E	<5%	1.702	1.914	0	0.46	1.073	0.733	0.850	0	0
245	ethyl benzoate	3.81E+01	E	<5%	1.580	1.465	0	0.46	1.214	0.689	0.850	0	0
246	diethyl phthalate	6.64E-02	EP	<10%	-1.178	-1.180	0	0.88	1.711	0.729	1.400	0	0
247	dimethyl phthalate	4.56E-01	E	<10%	-0.341	-0.255	0	0.88	1.429	0.78	1.410	0	0
248	n-propyl benzoate	1.15E+01	EP	<10%	1.062	1.062	0	0.46	1.354	0.675	0.800	0	0
249	ethyl mercaptan	7.03E+04	E	<3%	4.847	4.912	0	0.24	0.554	0.392	0.350	0	0
250	n-propyl mercaptan	2.06E+04	E	<3%	4.313	4.421	0	0.24	0.695	0.385	0.350	0	0
251	n-hexyl mercaptan	5.96E+02	E	<5%	2.775	2.951	0	0.24	1.118	0.361	0.350	0	0
252	n-nonyl mercaptan	1.54E+01	E	<5%	1.187	1.469	0	0.24	1.540	0.347	0.350	0	0
253	n-octyl mercaptan	6.12E+01	E	<5%	1.787	1.962	0	0.24	1.399	0.353	0.350	0	0
254	n-pentyl mercaptan	1.84E+03	E	<3%	3.265	3.440	0	0.24	0.977	0.369	0.350	0	0
255	n-heptyl mercaptan	1.77E+02	E	<5%	2.247	2.458	0	0.24	1.258	0.357	0.350	0	0
256	n-butyl mercaptan	6.19E+03	E	<3%	3.791	3.925	0	0.24	0.836	0.382	0.350	0	0
257	phenyl mercaptan	2.02E+02	E	<3%	2.305	2.363	0.09	0.16	0.880	1	0.800	0	0
258	2-butyne	9.41E+04	E	<1%	4.974	5.027	0	0.15	0.586	0.261	0.300	0	0
259	1-pentyne	5.81E+04	EP	<3%	4.764	4.738	0.12	0.12	0.727	0.172	0.230	0	0
260	1-hexyne	1.77E+04	E	<5%	4.248	4.245	0.12	0.1	0.868	0.166	0.230	0	0
261	1-octyne	1.75E+03	EP	<5%	3.244	3.258	0.12	0.1	1.150	0.155	0.230	0	0
262	1-nonyne	4.94E+02	EP	<10%	2.694	2.764	0.12	0.1	1.291	0.15	0.230	0	0
263	phenylethyne	1.08E+03	EP	<10%	3.032	2.958	0.12	0.24	0.912	0.679	0.580	0	0
264	1-heptyne	5.56E+03	E	<5%	3.745	3.753	0.12	0.1	1.009	0.16	0.230	0	0
265	trimethylamine	2.16E+05	E	<5%	5.334	5.161	0	0.67	0.631	0.14	0.200	0	0
266	triethylamine	9.13E+03	E	<5%	3.960	3.783	0	0.79	1.054	0.101	0.150	0	0
267	quinoline	1.11E+01	E	<3%	1.047	1.211	0	0.54	1.044	1.268	0.970	0	0
268	pyridine	2.77E+03	E	<1%	3.443	3.459	0	0.52	0.675	0.631	0.840	0	0
269	N,N-dimethylaniline	9.72E+01	E	<3%	1.988	1.580	0	0.41	1.098	0.957	0.840	0	0
270	2-methylpyridine	1.51E+03	E	<3%	3.179	3.134	0	0.58	0.816	0.598	0.750	0	0
271	pyrimidine	2.25E+03	EP	<3%	3.352	3.389	0	0.7	0.634	0.606	1.000	0	0
272	2,6-dimethylpyridine	7.73E+02	E	<3%	2.888	2.700	0	0.63	0.957	0.607	0.700	0	0
273	3-methylpyridine	8.10E+02	E	<3%	2.908	3.004	0	0.54	0.816	0.631	0.810	0	0
274	4-methylpyridine	7.68E+02	E	<3%	2.885	2.990	0	0.54	0.816	0.63	0.820	0	0
275	N-methylpyrrole	2.92E+03	E	<5%	3.466	3.465	0	0.31	0.718	0.559	0.790	0	0
276	acetonitrile	1.21E+04	E	<3%	4.084	4.393	0.07	0.32	0.404	0.237	0.900	0.258	0
277	propionitrile	6.31E+03	E	<3%	3.800	3.981	0.02	0.36	0.545	0.162	0.900	0.258	0
278	n-butyronitrile	2.60E+03	E	<3%	3.415	3.451	0	0.36	0.686	0.188	0.900	0.258	0
279	isobutyronitrile	4.36E+03	EP	<5%	3.640	3.551	0	0.36	0.686	0.142	0.870	0.258	0
280	valeronitrile	9.72E+02	E	<3%	2.988	2.964	0	0.36	0.827	0.177	0.900	0.258	0
281	benzonitrile	8.64E+01	E	<5%	1.936	1.830	0	0.33	0.871	0.742	1.110	0.258	0
282	hexanenitrile	3.79E+02	E	<5%	2.579	2.477	0	0.36	0.968	0.166	0.900	0.258	0
283	nitromethane	4.81E+03	E	<5%	3.682	4.061	0.06	0.31	0.424	0.313	0.950	0.322	0
284	nitroethane	2.76E+03	E	<5%	3.441	3.611	0.02	0.33	0.565	0.27	0.950	0.322	0
285	2-nitropropane	2.28E+03	E	<5%	3.358	3.220	0	0.33	0.706	0.216	0.920	0.322	0
286	1-nitropropane	1.35E+03	E	<5%	3.129	3.144	0	0.31	0.706	0.242	0.950	0.322	0
287	1-nitrobutane	4.73E+02	E	<5%	2.675	2.662	0	0.29	0.847	0.227	0.950	0.322	0
288	nitrobenzene	3.35E+01	E	<5%	1.526	1.512	0	0.28	0.891	0.871	1.110	0.322	0
289	m-nitrotoluene	1.42E+01	E	<10%	1.153	1.024	0	0.25	1.032	0.874	1.100	0.322	0
290	o-nitrotoluene	1.99E+01	E	<5%	1.299	1.018	0	0.27	1.032	0.866	1.110	0.322	0

Table S1. (cont.)

No.	Compound	$P_{\text{vap}}$ (Pa)	Source	Error	Predicted								
					$\log P_{\text{vap}}$	$\log P_{\text{vap}}$	A	B	V	E	S	$\lambda$	$\eta$
291	benzene	1.26E+04	E	<1%	4.102	4.131	0	0.14	0.716	0.61	0.520	-0.201	0
292	toluene	3.80E+03	E	<3%	3.580	3.642	0	0.14	0.857	0.601	0.520	-0.201	0
293	o-xylene	8.86E+02	E	<3%	2.948	3.009	0	0.16	0.998	0.663	0.560	-0.201	0
294	m-xylene	1.12E+03	E	<3%	3.049	3.116	0	0.16	0.998	0.623	0.520	-0.201	0
295	p-xylene	1.17E+03	E	<3%	3.068	3.128	0	0.16	0.998	0.613	0.520	-0.201	0
296	ethylbenzene	1.28E+03	E	<3%	3.107	3.143	0	0.15	0.998	0.613	0.510	-0.201	0
297	o-ethyltoluene	3.39E+02	E	<3%	2.530	2.505	0	0.18	1.139	0.68	0.550	-0.201	0
298	p-ethyltoluene	3.98E+02	E	<3%	2.600	2.624	0	0.18	1.139	0.63	0.510	-0.201	0
299	1,2,3-trimethylbenzene	2.16E+02	E	<3%	2.335	2.357	0	0.19	1.139	0.728	0.610	-0.201	0
300	1,2,4-trimethylbenzene	2.87E+02	E	<3%	2.458	2.493	0	0.19	1.139	0.677	0.560	-0.201	0
301	cumene	6.09E+02	E	<3%	2.784	2.687	0	0.16	1.139	0.602	0.490	-0.201	0
302	n-propylbenzene	4.64E+02	E	<3%	2.666	2.669	0	0.15	1.139	0.604	0.500	-0.201	0
303	1,2,3,4-tetramethylbenzene	4.42E+01	EP	<5%	1.645	1.705	0	0.19	1.280	0.794	0.660	-0.201	0
304	tert-butylbenzene	2.91E+02	E	<3%	2.463	2.167	0	0.16	1.280	0.619	0.490	-0.201	0
305	isobutylbenzene	2.65E+02	E	<3%	2.423	2.243	0	0.15	1.280	0.58	0.470	-0.201	0
306	n-butylbenzene	1.43E+02	E	<3%	2.156	2.159	0	0.15	1.280	0.6	0.510	-0.201	0
307	n-pentylbenzene	4.39E+01	E	<5%	1.643	1.666	0	0.15	1.421	0.594	0.510	-0.201	0
308	n-hexylbenzene	1.46E+01	EP	<5%	1.164	1.185	0	0.15	1.562	0.591	0.500	-0.201	0
309	n-octylbenzene	1.49E+00	E	<5%	0.174	0.230	0	0.15	1.844	0.579	0.480	-0.201	0
310	n-decylbenzene	1.51E-01	E	<5%	-0.822	-0.751	0	0.15	2.125	0.579	0.470	-0.201	0
311	styrene	8.17E+02	E	<1%	2.912	2.808	0	0.16	0.955	0.849	0.650	-0.201	0
312	?-methylstyrene	3.57E+02	EP	<5%	2.552	2.321	0	0.19	1.096	0.851	0.640	-0.201	0
313	1-methylnaphthalene	1.00E+01	E	<3%	1.002	1.077	0	0.2	1.226	1.344	0.900	-0.324	0
314	1-ethylnaphthalene	3.32E+00	E	<5%	0.521	0.577	0	0.2	1.367	1.371	0.880	-0.324	0
315	2-ethylnaphthalene	4.23E+00	E	<10%	0.627	0.593	0	0.2	1.367	1.331	0.900	-0.324	0
316	methylamine	3.53E+05	E	<3%	5.548	5.603	0.16	0.58	0.349	0.25	0.350	0	0.61
317	ethylamine	1.40E+05	E	<3%	5.145	5.109	0.16	0.61	0.490	0.236	0.350	0	0.61
318	allylamine	3.23E+04	P	<5%	4.509	4.426	0.16	0.58	0.588	0.35	0.490	0	0.61
319	n-propylamine	4.13E+04	E	<3%	4.616	4.622	0.16	0.61	0.631	0.225	0.350	0	0.61
320	isopropylamine	7.79E+04	E	<3%	4.891	4.719	0.16	0.61	0.631	0.181	0.320	0	0.61
321	n-butylamine	1.24E+04	E	<3%	4.093	4.123	0.16	0.61	0.772	0.224	0.350	0	0.61
322	isobutylamine	1.86E+04	E	<3%	4.269	4.192	0.16	0.63	0.772	0.198	0.320	0	0.61
323	sec-butylamine	2.37E+04	EP	<5%	4.374	4.225	0.16	0.63	0.772	0.17	0.320	0	0.61
324	tert-butylamine	4.95E+04	E	<5%	4.695	4.300	0.16	0.71	0.772	0.121	0.290	0	0.61
325	n-pentylamine	4.00E+03	EP	<3%	3.602	3.639	0.16	0.61	0.913	0.211	0.350	0	0.61
326	cyclohexylamine	1.34E+03	E	<5%	3.127	3.082	0.16	0.58	0.945	0.326	0.560	0	0.61
327	benzylamine	8.82E+01	EP	<5%	1.945	2.011	0.1	0.72	0.957	0.829	0.880	0	0.61
328	n-hexylamine	1.21E+03	E	<5%	3.084	3.155	0.16	0.61	1.054	0.197	0.350	0	0.61
329	n-heptylamine	4.45E+02	E	<5%	2.649	2.655	0.16	0.61	1.195	0.197	0.350	0	0.61
330	n-octylamine	1.34E+02	E	<5%	2.128	2.171	0.16	0.61	1.335	0.187	0.350	0	0.61
331	methanol	1.68E+04	E	<1%	4.226	4.334	0.43	0.47	0.308	0.278	0.440	0	2
332	ethanol	7.92E+03	E	<1%	3.899	4.077	0.37	0.48	0.449	0.246	0.420	0	2
333	1-propanol	2.81E+03	E	<3%	3.449	3.589	0.37	0.48	0.590	0.236	0.420	0	2
334	1-butanol	8.93E+02	E	<3%	2.951	3.104	0.37	0.48	0.731	0.224	0.420	0	2
335	1-pentanol	3.32E+02	EP	<3%	2.521	2.610	0.37	0.48	0.872	0.219	0.420	0	2
336	1-hexanol	1.03E+02	EP	<5%	2.014	2.120	0.37	0.48	1.013	0.21	0.420	0	2
337	1-heptanol	2.75E+01	EP	<3%	1.439	1.619	0.37	0.48	1.154	0.211	0.420	0	2
338	1-octanol	1.06E+01	E	<3%	1.024	1.134	0.37	0.48	1.295	0.199	0.420	0	2
339	1-nonanol	3.14E+00	E	<3%	0.497	0.644	0.37	0.48	1.435	0.193	0.420	0	2
340	1-decanol	1.14E+00	E	<3%	0.056	0.147	0.37	0.48	1.576	0.191	0.420	0	2
341	1-undecanol	4.26E-01	E	<5%	-0.371	-0.341	0.37	0.48	1.717	0.181	0.420	0	2
342	1-dodecanol	1.18E-01	E	<5%	-0.928	-0.834	0.37	0.48	1.858	0.175	0.420	0	2
343	allyl alcohol	3.39E+03	EP	<5%	3.530	3.523	0.38	0.48	0.547	0.342	0.460	0	2
344	2-chloroethanol	9.57E+02	E	<5%	2.981	2.535	0.47	0.57	0.572	0.419	0.590	0	2
345	2-methyl-1-propanol	1.40E+03	EP	<3%	3.146	3.157	0.37	0.48	0.731	0.217	0.390	0	2
346	2-methyl-1-butanol	4.86E+02	E	<3%	2.687	2.655	0.37	0.48	0.872	0.219	0.390	0	2
347	3-methyl-1-butanol	4.27E+02	E	<5%	2.630	2.687	0.37	0.48	0.872	0.192	0.390	0	2
348	benzyl alcohol	1.27E+01	E	<10%	1.102	1.037	0.33	0.56	0.916	0.803	0.870	0	2
349	dimethylamine	2.03E+05	E	<3%	5.308	5.451	0.08	0.66	0.490	0.189	0.300	0	0
350	diethylamine	3.14E+04	E	<3%	4.497	4.493	0.08	0.69	0.772	0.154	0.300	0	0
351	piperidine	4.28E+03	E	<3%	3.632	3.822	0.1	0.69	0.804	0.422	0.460	0	0
352	di-n-propylamine	3.61E+03	EP	<10%	3.558	3.528	0.08	0.69	1.054	0.124	0.300	0	0

**Table S1.** (cont.)

No.	Compound	$P_{\text{vap}}$ (Pa)	Source	Error	Predicted								
					$\log P_{\text{vap}}$	$\log P_{\text{vap}}$	$A$	$B$	$V$	$E$	$S$	$\lambda$	$\eta$
353	diisopropylamine	1.06E+04	E	<5%	4.024	3.702	0.08	0.73	1.054	0.523	0.240	0	0
354	di-n-butylamine	3.65E+02	E	<3%	2.562	2.552	0.08	0.69	1.335	0.107	0.300	0	0
355	2-propanol	6.05E+03	EP	<3%	3.782	4.034	0.33	0.56	0.590	0.212	0.360	0	1.43
356	2-butanol	2.41E+03	E	<3%	3.383	3.528	0.33	0.56	0.731	0.217	0.360	0	1.43
357	3-methyl-2-butanol	1.21E+03	E	<5%	3.082	3.101	0.33	0.56	0.872	0.194	0.330	0	1.43
358	3-pentanol	1.09E+03	E	<5%	3.037	3.027	0.33	0.56	0.872	0.218	0.360	0	1.43
359	2-pentanol	8.22E+02	E	<3%	2.915	3.054	0.33	0.56	0.872	0.195	0.360	0	1.43
360	4-methyl-2-pentanol	7.02E+02	E	<5%	2.846	2.633	0.33	0.56	1.013	0.167	0.330	0	1.43
361	2-hexanol	3.34E+02	E	<5%	2.524	2.564	0.33	0.56	1.013	0.187	0.360	0	1.43
362	2-heptanol	1.27E+02	EP	<5%	2.103	2.063	0.33	0.56	1.154	0.188	0.360	0	1.43
363	2-octanol	3.23E+01	E	<3%	1.509	1.598	0.33	0.56	1.295	0.158	0.360	0	1.43
364	1-phenylethanol	2.37E+01	E	<5%	1.375	0.929	0.3	0.66	1.057	0.784	0.830	0	1.43
365	pyrrole	1.10E+03	E	<3%	3.040	3.452	0.41	0.29	0.577	0.613	0.730	0	1.27
366	aniline	9.01E+01	E	<3%	1.955	1.912	0.26	0.41	0.816	0.955	0.960	0	1.27
367	o-chloroaniline	3.30E+01	E	<5%	1.519	1.580	0.25	0.31	0.939	1.033	0.920	0	1.27
368	m-chloroaniline	8.79E+00	E	<5%	0.944	1.225	0.3	0.3	0.939	1.053	1.100	0	1.27
369	N-methylaniline	5.98E+01	E	<3%	1.776	1.665	0.17	0.43	0.957	0.948	0.900	0	1.27
370	o-toluidine	3.47E+01	E	<5%	1.540	1.475	0.23	0.45	0.957	0.966	0.920	0	1.27
371	m-toluidine	2.58E+01	E	<5%	1.412	1.453	0.23	0.45	0.957	0.946	0.950	0	1.27
372	2-methyl-2-propanol	5.58E+03	E	<3%	3.747	3.745	0.31	0.6	0.731	0.18	0.310	0	1.27
373	2-methyl-2-butanol	2.23E+03	E	<3%	3.347	3.377	0.32	0.49	0.872	0.194	0.300	0	1.27
374	m-cresol	1.85E+01	E	<3%	1.267	1.438	0.57	0.34	0.916	0.822	0.880	0	1.27
375	m-ethylphenol	6.98E+00	E	<5%	0.844	0.862	0.55	0.37	1.057	0.81	0.910	0	1.27
376	o-ethylphenol	2.07E+01	E	<5%	1.317	0.995	0.52	0.37	1.057	0.831	0.840	0	1.27

Explanation of column headings: Values of  $P_{\text{vap}}$  are calculated from DIPPR equation 101, using the constants given for a specific compound. The source of the constants is experimental (E), predicted (P), or a combination of the two (EP). The error is the maximum percent error of the resulting  $P_{\text{vap}}$  values as determined by DIPPR. Predicted  $\log P_{\text{vap}}$  is the value of  $\log P_{\text{vap}}$  calculated using equation 6 and the solute parameters  $A$ ,  $B$ ,  $V$ ,  $E$ ,  $S$ ,  $\lambda$ , and  $\eta$ . The sources of the parameters  $A$ ,  $B$ ,  $V$ ,  $E$ , and  $S$  are given in the text, and the values of  $\lambda$ , and  $\eta$  are taken from the manuscript.

**Table S2.** Solute parameters estimated from molecular structure\*

Compound Class	$A$	$B$	$S$
Alkane	0	0	0
Cycloalkane	0	0	0.13
Acyclic Alkene	0	0.08	0.12
Cycloalkene	0	0.03	0.08
Conjugated Diene	0	0.11	0.23
Alkylbenzene (note $\lambda$ also)	0	0.16	0.53
Dialkyl Sulfide	0	0.30	0.38
Dialkyl Disulfide	0	0.28	0.46
Dialkyl Ether	0	0.44	0.24
Aliphatic Aldehyde	0	0.44	0.65
Aliphatic Ketone	0	0.51	0.67
Aliphatic Ester	0	0.44	0.60
Aliphatic Nitrile (note $\lambda$ also)	0.02	0.35	4.90
Alkylmercaptan	0	0.24	0.35
Terminal Alkyne	0.12	0.12	0.23
Internal Alkyne	0	0.15	0.00
Primary Aliphatic Amine (note $\eta$ also)	0.16	0.62	0.35
Secondary Aliphatic Amine	0.08	0.69	0.29
Tertiary Aliphatic Amine	0	0.73	0.18
Primary Alcohol (note $\eta$ also)	0.37	0.48	0.42
Secondary Alcohol (note $\eta$ also)	0.33	0.56	0.35
Tertiary Alcohol (note $\eta$ also)	0.32	0.55	0.31
Alkyl naphthalene (note $\lambda$ also)	0	0.20	0.89

\* $E$  values for molecules with a particular functional group tend to decrease with increasing alkyl substitution because the difference between the compound's index of refraction and the index of refraction of an alkane with the same molecular volume tends to decrease as the compound becomes more alkane-like. Thus  $E$  values may be interpolated from values of homologous compounds in Table S1 above if a sufficient range of values is available. This was done for the compounds in Table S3 except for the higher molecular weight trialkylamines, for which  $E$  values were calculated as indicated in Lima, G. A. R. Ph.D. Thesis, University of São Paulo, Brazil, 2000.



**Table S3.** Solute parameters and  $\log P_{\text{vap}}$  values used to prepare Figure 5

No. Compound	$P_{\text{vap}}$ (Pa)	Source	Error	A	B	V	E	S+ $\lambda$	$\eta^*A*B$	$\log P_{\text{vap}}$	Predicted $\log P_{\text{vap}}$
1 propylcyclopentane	1.647E+03	EP	< 3%	0	0	1.127	0.225	0.100	0	3.217	3.456
2 5-methyl-1-hexene	1.034E+04	P	< 5%	0	0.078	1.052	0.092	0.080	0	4.015	3.908
3 trans-2-pentene	6.743E+04	E	< 1%	0	0.078	0.770	0.092	0.080	0	4.829	4.907
4 2-ethyl-1-butene	2.338E+04	E	< 3%	0	0.078	0.911	0.092	0.080	0	4.369	4.407
5 2,4,4-trimethyl-2-pentene	4.786E+03	E	< 3%	0	0.078	1.193	0.092	0.080	0	3.680	3.408
6 1-tridecene	7.334E+00	E	< 3%	0	0.078	1.897	0.092	0.080	0	0.865	0.912
7 6-methyl-1-heptene	3.305E+03	P	< 5%	0	0.078	1.193	0.092	0.080	0	3.519	3.408
8 1-heptadecene	6.924E-02	E	< 5%	0	0.078	2.461	0.092	0.080	0	-1.160	-1.086
9 trans-1,3-pentadiene	5.482E+04	E	< 1%	0	0.113	0.727	0.352	0.230	0	4.739	4.528
10 trans,trans-2,4-hexadiene	1.171E+04	E	< 1%	0	0.113	0.868	0.352	0.230	0	4.069	4.028
11 1,2-dichlorobutane	2.165E+03	EP	< 5%	0.1	0.11	0.917	0.680	0.220	0	3.336	3.488
12 2,3-dichlorobutane	2.701E+03	EP	< 10%	0.1	0.11	0.917	0.680	0.220	0	3.431	3.488
13 isopropyl iodide	9.493E+03	E	< 5%	0	0.15	0.654	0.634	0.400	0	3.977	4.201
14 m-ethyltoluene	4.243E+02	E	< 3%	0	0.16	1.139	0.640	0.316	0	2.628	2.602
15 sec-butylbenzene	2.241E+02	E	< 3%	0	0.16	1.280	0.640	0.316	0	2.350	2.102
16 m-cymene	2.322E+02	E	< 3%	0	0.16	1.280	0.640	0.316	0	2.366	2.102
17 m-diethylbenzene	1.604E+02	E	< 3%	0	0.16	1.280	0.640	0.316	0	2.205	2.102
18 p-diisopropylbenzene	3.281E+01	E	< 3%	0	0.16	1.562	0.640	0.316	0	1.516	1.104
19 heptylbenzene	4.803E+00	EP	< 5%	0	0.16	1.703	0.640	0.316	0	0.681	0.604
20 undecylbenzene	4.596E-02	E	< 3%	0	0.16	2.266	0.640	0.316	0	-1.338	-1.393
21 methyl propyl sulfide	6.786E+03	E	< 3%	0	0.3025	0.836	0.381	0.380	0	3.832	3.880
22 ethyl octyl sulfide	1.213E+01	E	< 3%	0	0.3025	1.681	0.381	0.380	0	1.084	0.884
23 dipropyl disulfide	1.039E+02	E	< 3%	0	0.28	1.281	0.683	0.460	0	2.017	1.829
24 methyl butyl sulfide	2.079E+03	E	< 3%	0	0.3025	0.977	0.381	0.380	0	3.318	3.381
25 di-sec-butyl ether	2.144E+03	EP	< 5%	0	0.437	1.295	0.030	0.243	0	3.331	2.871
26 methyl ethyl ether	1.959E+05	E	< 5%	0	0.437	0.590	0.030	0.243	0	5.292	5.368
27 butyl isopropyl ether	3.462E+03	EP	< 5%	0	0.437	1.154	0.030	0.243	0	3.539	3.371
28 dihexyl ether	6.144E+00	EP	< 5%	0	0.437	1.858	0.030	0.243	0	0.788	0.874
29 methyl butyl ether	1.829E+04	EP	< 5%	0	0.437	0.872	0.030	0.243	0	4.262	4.369
30 ethyl propyl ether	2.407E+04	E	< 5%	0	0.437	0.872	0.030	0.243	0	4.381	4.369
31 dipentyl ether	1.142E+02	EP	< 5%	0	0.437	1.576	0.030	0.243	0	2.058	1.873
32 methyl pentyl ether	5.694E+03	EP	< 5%	0	0.437	1.013	0.030	0.243	0	3.755	3.870
33 butyl ethyl ether	7.367E+03	EP	< 3%	0	0.437	1.013	0.030	0.243	0	3.867	3.870
34 ethyl hexyl ether	6.431E+02	EP	< 10%	0	0.437	1.295	0.030	0.243	0	2.808	2.871
35 2-ethylhexanal	2.615E+02	EP	< 5%	0	0.438	1.252	0.171	0.654	0	2.417	2.234
36 3-methylhexanal	8.033E+02	EP	< 5%	0	0.438	1.111	0.171	0.654	0	2.905	2.733
37 decanal	1.271E+01	E	< 5%	0	0.438	1.533	0.171	0.654	0	1.104	1.235
38 dodecanal	1.649E+00	E	< 5%	0	0.438	1.815	0.171	0.654	0	0.217	0.236
39 3-methyl-2-pentanone	2.568E+03	E	< 5%	0	0.509	0.970	0.130	0.667	0	3.410	3.261
40 3-heptanone	5.619E+02	E	< 10%	0	0.509	1.111	0.130	0.667	0	2.750	2.762
41 ethyl isopropyl ketone	2.733E+03	E	< 10%	0	0.509	0.970	0.130	0.667	0	3.437	3.261
42 octyl formate	8.125E+01	EP	< 5%	0	0.438	1.451	0.093	0.597	0	1.910	1.704
43 nonyl formate	2.278E+01	EP	< 10%	0	0.438	1.592	0.093	0.597	0	1.358	1.205
44 sec-butyl acetate	2.961E+03	EP	< 5%	0	0.438	1.028	0.093	0.597	0	3.471	3.202
45 butyl propionate	5.970E+02	EP	< 5%	0	0.438	1.169	0.093	0.597	0	2.776	2.703
46 propyl isobutyrate	8.874E+02	EP	< 5%	0	0.438	1.169	0.093	0.597	0	2.948	2.703
47 butyl valerate	7.847E+01	EP	< 10%	0	0.438	1.451	0.093	0.597	0	1.895	1.704
48 ethyl isovalerate	1.073E+03	EP	< 5%	0	0.438	1.169	0.093	0.597	0	3.030	2.703
49 nonyl acetate	6.663E+00	EP	< 10%	0	0.438	1.733	0.093	0.597	0	0.824	0.705
50 decyl acetate	1.553E+00	E	< 25%	0	0.438	1.874	0.093	0.597	0	0.191	0.206
51 hexyl formate	3.559E+02	EP	< 5%	0	0.438	1.169	0.093	0.597	0	2.551	2.703
52 heptyl formate	1.699E+02	EP	< 5%	0	0.438	1.310	0.093	0.597	0	2.230	2.203
53 t-butanethiol	2.416E+04	E	< 3%	0	0.24	0.836	0.372	0.350	0	4.383	3.937
54 2-methylpropanethiol	9.275E+03	E	< 3%	0	0.24	0.836	0.372	0.350	0	3.967	3.937
55 hexanethiol	5.961E+02	E	< 5%	0	0.24	1.118	0.372	0.350	0	2.775	2.938
56 2-propanethiol	3.694E+04	E	< 3%	0	0.24	0.695	0.372	0.350	0	4.567	4.436
57 3-hexyne	1.213E+04	EP	< 5%	0	0.15	0.868	0.261	0.300	0	4.084	4.028
58 2-hexyne	1.067E+04	EP	< 3%	0	0.15	0.868	0.261	0.300	0	4.028	4.028
59 1-decyne	1.651E+02	EP	< 10%	0.12	0.117	1.432	0.166	0.233	0	2.218	2.243
60 nonylamine	4.345E+01	E	< 5%	0.16	0.616	1.477	0.208	0.354	0.06	1.638	1.639
61 decylamine	1.329E+01	E	< 5%	0.16	0.616	1.617	0.208	0.354	0.06	1.123	1.140
62 dipentylamine	2.042E+01	EP	< 10%	0.08	0.692	1.617	0.125	0.288	0	1.310	1.548

**Table S3.** (cont.)

No.Compound	$P_{\text{vap}}$ (Pa)	Source	Error	A	B	V	E	$S+\lambda$	$\eta^*A^*B$	$\log P_{\text{vap}}$	Predicted $\log P_{\text{vap}}$
63 2-methyl-2-butanamine	1.349E+04	EP	< 5%	0	0.73	0.913	0.121	0.354	0	4.130	3.950
64 butyldimethylamine	7.062E+03	EP	< 10%	0	0.73	1.054	0.121	0.180	0	3.849	3.716
65 tributylamine	1.244E+01	EP	< 5%	0	0.73	1.899	0.020	0.180	0	1.095	0.836
66 2-methylpentanol	1.951E+02	E	< 5%	0.37	0.48	1.013	0.210	0.420	0.355	2.290	2.120
67 3-methylpentanol	1.285E+02	E	< 5%	0.37	0.48	1.013	0.210	0.420	0.355	2.109	2.120
68 2-methylhexanol	8.598E+01	EP	< 5%	0.37	0.48	1.154	0.208	0.420	0.355	1.934	1.625
69 5-methylhexanol	5.143E+01	EP	< 10%	0.37	0.48	1.154	0.211	0.420	0.355	1.711	1.619
70 8-methylnonanol	2.753E+00	EP	< 5%	0.37	0.48	1.576	0.191	0.420	0.355	0.440	0.147
71 2-nonanol	1.718E+01	EP	< 10%	0.33	0.56	1.435	0.193	0.420	0.259	1.235	0.989
72 3-methyl-3-pentanol	1.334E+03	E	< 10%	0.32	0.49	1.013	0.194	0.300	0.188	3.125	2.920
73 nonylphenol	3.143E-03	EP	< 10%	0.55	0.37	2.043	0.810	0.910	0.244	-2.503	-2.579
74 1-butyl-naphthalene	4.378E-01	EP	< 10%	0	0.2	1.649	1.371	0.541	0	-0.359	-0.401
75 1-propylnaphthalene	1.760E+00	E	< 10%	0	0.2	1.508	1.371	0.541	0	0.246	0.099
76 1-pentylnaphthalene	1.606E-01	EP	< 10%	0	0.2	1.790	1.371	0.541	0	-0.794	-0.900

**Table S4.** Statistical data for LSER correlations

Equations 2, 4, 5, and 6 are reproduced below. The uncertainties shown for each intercept and coefficient are the standard deviations of those values. Below each equation are shown the partial  $F$  values for the parameter immediately above the value indicated.

Equation 2					
$\log P_{\text{vap}} = (7.78 \pm 0.04) - (3.45 \pm 0.03) V - (0.93 \pm 0.04) E - (1.70 \pm 0.04) S$					
Partial $F$ values for the coefficients:		10497	456	1506	
Equation 4					
$\log P_{\text{vap}} = (7.86 \pm 0.03) - (3.54 \pm 0.03) V - (1.17 \pm 0.03) E - (1.52 \pm 0.03) (S + \lambda)$					
Partial $F$ values for the coefficients:		18236	1474	2764	
Equation 5					
$\log P_{\text{vap}} = (7.92 \pm 0.04) - (3.58 \pm 0.03) V - (1.15 \pm 0.04) E - (1.53 \pm 0.04) (S + \lambda) - (5.75 \pm 0.17) (A \times B)$					
Partial $F$ values for the coefficients:		13654	948	1784	1098
Equation 6					
$\log P_{\text{vap}} = (7.86 \pm 0.03) - (3.54 \pm 0.02) V - (1.17 \pm 0.03) E - (1.52 \pm 0.03) (S + \lambda) - (3.64 \pm 0.08) (\eta \times A \times B)$					
Partial $F$ values for the coefficients:		21270	1533	2782	1954

**Table S5.** Correlation matrix for solute parameters

The following table shows the cross-correlation of the solute parameters for all 376 compounds in the data set used to generate equation 6:

	A	B	V	E	S
A	1				
B	0.370683	1			
V	-0.14024	-0.21814	1		
E	0.095105	0.083291	-0.17908	1	
S	0.108824	0.553608	-0.28583	0.658822	1