A Quantitative Structure Property Relation Correlation of the Dielectric Constant for Organic Chemicals

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The dielectric constant (ε) or relative static permittivity of a material represents the capacitance of the material relative to a vacuum and is important in many industrial applications. Nevertheless, accurate experimental values are often unavailable, and current prediction methods lack accuracy and are often unreliable. Reported here is the development and testing of a new QSPR (quantitative structure property relation) correlation of ε for organic chemicals. On the basis of the regression analysis and tests of the correlation in prediction mode, the average absolute percent error is expected to be less than 3 % when applied to hydrocarbons and nonpolar compounds and less than 18 % when applied to polar compounds with ε values ranging from 1.0 to 50.0. The correlation requires values for the dipole moment, solubility parameter, van der Waals area, and refractive index. We show also that density functional calculations of the dipole moment using B3LYP/6-311+G(3df,2p) can be used in the ε correlation, when experimental values are unavailable, with little decrease in accuracy of the predicted values.

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1. Introduction

The dielectric constant (ε, DC) or relative static permittivity represents the capacitance of a material relative to that of a vacuum. The capacitance enhancement of a dielectric material arises from the orientation of charges within the material in response to an applied electrostatic field. Charge orientation is often thought of in terms of two constituent polarization modes: orientation or rotation polarization in which molecules with permanent dipoles experience an increase in dipole alignment from the thermally driven random orientation, and distortion polarization in which atomic and electronic polarization occur because of the effect of the applied field on bond lengths, bond angles, and electron distribution within the molecule. Values of ε therefore characterize the polarizability of the material. Because they are a measure of polarizability, ε values have become important in industrial design processes not only for typifying the dielectric nature of the material but also for providing solubility and separation information useful in separation designs, chemical equilibrium, and chemical reactivity analysis.

While experimentally determined ε values are available for the most commonly used chemicals, there are a large number of industrially important chemicals for which no measured value is available in the literature. This is particularly apparent to us as principal investigators for the DIPPR 801 Pure Chemical Database.[1] A hallmark of this database is "completeness," meaning that recommended constant property values or temperature-dependent correlations are provided in the database for all 45 properties of each chemical included in the database. This completeness philosophy requires that recommendations of property values be made from accurate, reliable prediction techniques when experimental data are not available. In the case of a DC, experimental data are available for only about 30 % of the chemicals in the database. Unfortunately, most available prediction methods for ε are rather rudimentary and often fail significantly (with errors of 100 % or more) for strongly polar compounds. Theoretical approaches, such as the Clausius−Mosotti[2] equation based on Deby's dielectric theory,[3] are generally useful only for dilute gases and some liquids of limited polarity. The Onsager equation[4] and the Kirkwood[5,6] extension provide improvement for some polar fluids, but their overall reliability is poor. The Kirkwood theory contains a correlation parameter, g, which is a measure of the local ordering that cannot be calculated directly nor has a correlation been developed for it. The poor predictive behavior of these statistical mechanics methods suggests that orientational polarization effects have not been fully accounted for, particularly for fluids where stronger association is possible, as is the case with strongly hydrogen-bonding liquids such as water or alcohols. It is also likely that the inability to correlate the correlation parameter g in the Kirkwood theory is due to multiple orientation and distortion polarization effects that are lumped into this parameter because of the difficulty in treating them explicitly.

Correlations have also been developed to relate ε to other measurable properties. The relationships between ε and the refractive index for nonpolar molecules and between ε and dipole moment (μ) are well-known and arise out of the previously mentioned theories. However, additional empirical correlations have also been found. For example, there appears to be a strong relationship between surface tension and ε that has been exploited in fairly simple correlations between these two properties by Papazian[7] and Holmes.[8] Paruta and coworkers[9] found a strong correlation between the solubility parameter and ε as did Gorman and Hall.[10] These correlations were developed for relatively small numbers of compounds, often for specific types of compounds. For example, the Paruta correlation was found to be particularly useful for hydrogen bonding chemicals. These correlations provide useful but approximate estimations of ε, but they do not constitute accurate predictive equations.

Quantitative structure property relations (QSPR) have also been developed that correlate molecular descriptors with ε. In

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the past decade, three such QSPR models have been developed in the literature. Schweitzer and Morris[11] used neural networks to build 70 000 models for a data set of 497 compounds ranging in ε values from 1 to 40. The best 119 models included 6 to 12 descriptors, but the best correlations still had relative errors larger than 100 % for 37 compounds and larger than 50 % for 115 compounds. Cocchi et al.[12] used a training set of only 23 compounds to develop a three-parameter QSPR model with a root-mean-squared (rms) error of 2.26, which then produced a rms of 4.65 for a test set consisting of 20 compounds. More recently, Sild and Karelson[13] developed a QSPR correlation for ε and for the Kirkwood function that uses six molecular descriptors. The average error of their correlation was 23.3 % for their training set of 155 compounds ranging in ε values from 1.87 to 46.5. Training sets for these methods were relatively small, and extrapolation reliability generally decreases with smaller training sets and larger numbers of parameters.

The DIPPR 801 database provides a convenient and powerful tool for QSPR development as over 154 molecular descriptors have been precalculated and tabulated in the database in addition to the collection of experimental property data available. In this work, ε data from the DIPPR 801 database have been used to develop a new QSPR correlation for ε using the available properties and molecular descriptors. In doing so, the guiding philosophy was to use only descriptors with a strong independent correlation to ε, minimize the number of descriptors in the correlation, and choose descriptors that rationally relate to the molecular physics presumed to underpin ε.

2. DC Correlation

2.1. Development of the Correlation. Training data for the correlation, obtained from the DIPPR 801 database, included 686 compounds with experimental ε values ranging from 1 to 50. A few experimental values greater than 50 were available, ranging up to 179, but these were scattered over such a wide range with very few representative compounds that they were not included in the training data.

The training data were divided into two sets. Set 1 consisted of all hydrocarbons and molecules with a structural symmetry that produces no dipole moment. Nominally this group can be thought of as low polarity. This training set included 167 chemicals with ε values ranging from 1.76 to 3.35. Set 2 included all other organic molecules, and it can be thought of nominally as more polar, though the dipole moment of some molecules in this group is small because of molecular structure. Training set 2 included the remaining 519 chemicals covering a wide range of chemical functionality.

A total of 315 molecular descriptors and physical properties were available either in the DIPPR 801 database (the NIST site contains computational results generated by numerous researches using various levels of theory and basis set sizes) or as directly generated using CODESSA[14] (comprehensive descriptors for structural and statistical analysis). In both cases, the descriptors are based on the optimized molecular geometry and electron distributions obtained using Gaussian98[15] HF/6-31G* calculations. Many molecular descriptors are not extremely sensitive to the model chemistry used to generate them, and this is particularly true of the descriptors selected in the final correlation. The available molecular descriptors included structural, topological, electronic, geometric, and chemical groups.

A stepwise multiple-linear-regression analysis was applied to select the most significant descriptors for a linear QSPR model using Tsar QSAR,[16] a fully integrated analysis package for investigation of quantitative structure−activity relationships (QSAR). Colinearity and cross correlation coefficients in Tsar QSAR were used to reduce the original 315 descriptor set to fewer than 20. In doing so, tightly coupled parameters often gave similar correlation coefficients. In this case, the descriptor with the greatest perceived physical significance and general availability was retained.

Table 1. Group Contribution Values, G_i, for Molecules Containing Oxygen Atoms

group	example	G_i	group	example	G_i
[S,N,P]=O	thionyl chloride	0.2879	−OH	alcohol	0.2230
>C=O	ketones	0.3615	−OH	phenol	0.0990
>C=O ring	2-pyrrolidone	0.0075	−OH ($C < 5$)[a]	ethanol	0.3348
−COO−	esters	−0.0650	CHO	aldehydes	0.1617
−COOH	acids	−0.5900			

[a] Applied in addition to regular −OH group for molecules with fewer than 5 C atoms.

Table 2. Correlation Coefficients for Equation 1

	C_0	C_1	C_2	C_3	C_4
nonpolar	−0.1694	0.1283	0	$2.8251\cdot10^{-5}$	0.2150
polar	−0.3416	0.5239	$4.072\cdot10^{8}$	$7.408\cdot10^{-5}$	−0.3248

The final independent variables were chosen on the basis of (1) sensitivity of ε to the descriptor, (2) a perceived direct relation of the descriptor to the molecular nature of the DC, and (3) ready availability of the descriptor values to users of the correlation. For example, ε was found to be strongly correlated colinearly to the van de Waals surface area and the Kier−Hall index of order zero, but the former was chosen because of its availability in the main tables of the DIPPR 801 database. The strongest correlation was found between ε and the dipole moment (μ), solubility parameter (δ), van der Waals area (A_{vdw}), and refractive index (n). The refractive index and dipole moment are prominent in the theoretical equations for the DC and would be expected to be important in its correlation.

2.2. Results and Analysis. The final correlation contains four molecular descriptors or properties supplemented with nine specific group contribution values for molecules containing oxygen atoms. Chemicals without oxygen atoms were well-correlated with the four descriptors. We speculate that orientation-specific interactions and associations (e.g., hydrogen bonds) that are more prevalent in oxygen-containing molecules may account for the necessity of adding group-specific interactions to the correlation for these compounds.

The general correlation can be written as

$$\ln \varepsilon = C_0 + C_1\left(\frac{\mu}{\mathrm{D}}\right) + C_2\left(\frac{A_{\mathrm{vdw}}}{\mathrm{m^2\cdot kmol^{-1}}}\right)^{-1} + C_3\left(\frac{\delta}{\mathrm{J^{1/2}\cdot m^{3/2}}}\right) + C_4 n^2 + \sum_{i}^{\text{O groups}} \frac{G_i}{k_i} \qquad (1)$$

in which G_i are the contributions for the oxygen containing group i, the values of which are given in Table 1, and k_i is the number of instances of group i in the molecule. Obviously, the group contribution term in eq 1 is to be used only when $k_i > 0$, that is, when there is at least one group i present in the molecule. Refractive index, n, values are for sodium D line incident light (0.5896 μm). The dipole moment values used from the DIPPR 801 database are gas-phase values or those measured in benzene at 298.15 K, which tend to be closer to the gas-phase values than those measured in other solvents.

Values of the correlation coefficients C_i to be used in eq 1 are given in Table 2. Separate regressions were performed on the two training sets yielding different values for the C_i to be used for nonpolar compounds or hydrocarbons than those for

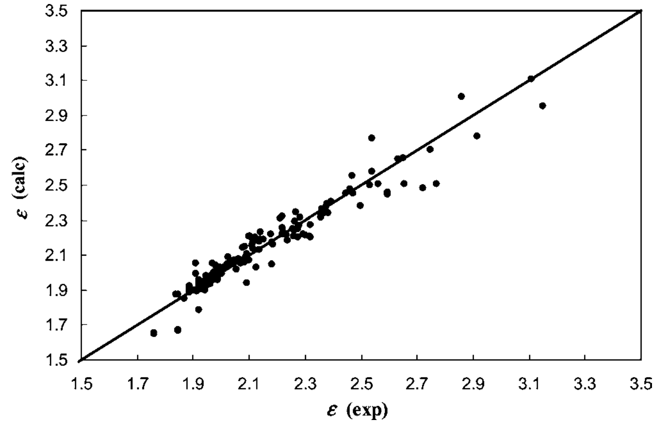

Figure 1. Calculated, ε (calc), and experimental, ε (exp), values for training set 1.

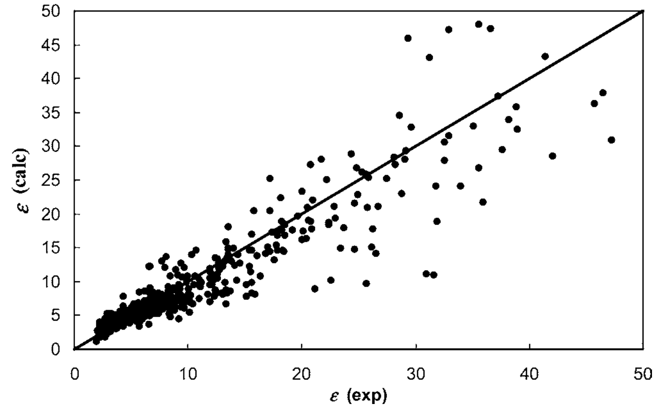

Figure 2. Calculated, ε (calc), and experimental, ε (exp), values for training set 2.

other organic polar compounds. Note that $C_2 = 0$ for training set 1 fluids so that the correlation for hydrocarbon and nonpolar compounds is only a function of the three descriptors: n, μ, and δ, and it can be written as

$$\ln \varepsilon = C_0 + C_1\left(\frac{\mu}{\mathrm{D}}\right) + C_3\left(\frac{\delta}{\mathrm{J}^{1/2}\cdot\mathrm{m}^{3/2}}\right) + C_4 n^2 \quad \text{(nonpolar or hydrocarbon)} \qquad (2)$$

This three-parameter correlation fits the training set 1 data with the cross-validated R^2 value of 0.9459, an average absolute deviation (AAD) of 0.07, and an average absolute percent deviation (AAPD) of 2.96 %. The correlation of calculated and experimental values is shown in Figure 1.

The correlation given in Equation 1 represents the 519 compounds in training set 2 (polar, nonhydrocarbon molecules) well with a few exceptions. The uncertainty in the experimental data is significantly higher for these compounds, and our critical examination of the data coupled with the inability of the wide range of possible descriptors to significantly improve the correlation suggests that we are approaching the limit of data accuracy. Figure 2 shows the final correlation of calculated and experimental values using eq 1, which yielded a cross-validated R^2 value of 0.8416, an AAD of 2.05, and an AAPD of 17.8 %.

There appear to be several outliers around $\varepsilon = 31$. These are for 1,4-butanediol ($\varepsilon = 31.9$), 3-chloro-1,2-propanediol ($\varepsilon = 31$), and ethyl cyanoacetate ($\varepsilon = 31.62$). These compounds have multiple polar groups, two —OH groups in the case of the two diol compounds and a cyano and an ester group in the case of ethyl cyanoacetate. Many of the chemicals with high DC values also have multiple polar groups within them. Unfortunately, the current correlation cannot account for potential internal group–group interactions and other induction effects that are likely to affect the molecular charge distribution and polarizability of the molecule. Available experimental data and their accuracy are currently inadequate to further refine the correlation to include such effects. Likely such a refinement would require a substantial set of group-contribution parameters determined from few experimental data which decreases the reliability of the use of the correlation to predict unknown ε values.

A breakdown of the correlation results, Figure 3, shows that 55 % (283 compounds) of the ε values in the polar (set 2) training set are within 1.0 of the experimental values and 73 % (379 compounds) are within 2.0 of the experimental values. In terms of percentage error, eq 1 correlates 45 % of the compounds within 10 % of the experimental values; 81 % are correlated within 30 % of the experimental values.

It should also be mentioned that experimental dipole moments were not available in the DIPPR 801 database for 74 of the chemicals in the test set. In these cases, values of μ were calculated with density functional theory in Gaussian03[17] using B3LYP/6-311+G(3df,2p). Comparison data in an online repository (the NIST site contains computational results generated by numerous researches using various levels of theory and basis set sizes) of ab initio results established by NIST[18] shows that B3LYP/6-311+G(3df,2p) calculations are the most reliable of the commonly used ab initio and density functional theory methods for calculating μ. In our own work, we found an AAPD

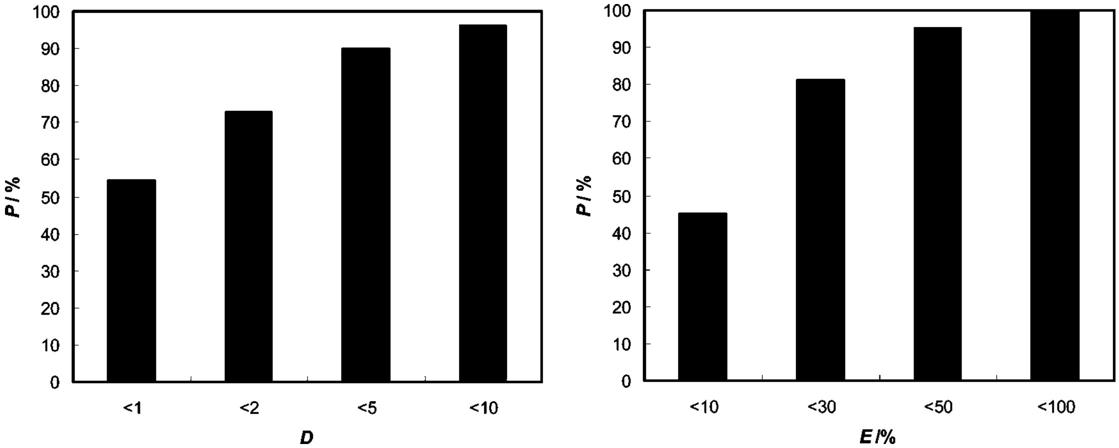

Figure 3. Percent (P) of the compounds in the polar (set 2) training set for which the correlation gives absolute (D) and percent (E) deviations in the categories shown.

Table 3. Test Set Compounds and Their Descriptor and ε Values

compound	μ D	A_{vdw} 10^8 $\mathrm{m^2 \cdot kmol^{-1}}$	δ 10^3 $\mathrm{J^{1/2} \cdot m^{3/2}}$	n	$\varepsilon_{\mathrm{calc}}$	$\varepsilon_{\mathrm{exp}}$	diff. %
ethyl methyl carbonate	0.6356	8.39	17.55	1.378	2.99	2.985	0.13
1-chlorohexane	2.4547	10.69	15.46	1.4199	6.14	6.104	0.66
butyl phenyl ether	1.6366	10.75	15.67	1.497	3.77	3.734	1.04
N,*N*-dibutylformamide	4.2496	12.01	15.78	1.443	17.77	18.4	–3.40
propyl chlorocarbonate	3.3628	8.84	17.36	1.411	11.65	11.2	4.01
2-methyl-2-butanethiol	1.7606	7.71	15.42	1.441	4.84	5.087	–4.88
methyl heptanoate	1.7035	9.14	15.27	1.41237	4.12	4.355	–5.49
ethyl hexanoate	1.7912	10.49	15.21	1.406	4.07	4.45	–8.44
ethyl 4-pyridinecarboxylate	2.8681	9.67	17.74	1.501	8.16	8.95	–8.83
N,*N*-dibutylacetamide	3.9905	13.36	15.00	1.447	17.23	19.1	–9.80
4-ethylpyridine	2.8518	7.47	17.78	1.498	9.83	10.98	–10.43
cyclohexyl butanoate	1.9079	7.02	15.43	1.445	5.14	4.58	12.27
2,2-dimethylpropanol	2.8616	8.73	16.46	1.3794	10.88	9.051	20.22
tribromoacetaldehyde	1.6619	8.64	19.79	1.621	5.90	7.6	–22.38
octanenitrile	4.5214	13.52	16.47	1.42	18.06	13.9	29.91
ethyl 2-bromopropanoate	2.4502	9.88	17.10	1.446	6.53	9.4	–30.53
1-fluorooctane	2.2446	12.72	15.12	1.389	5.20	3.89	33.57
cyclohexyl propanoate	2.0142	5.67	15.85	1.4425	6.45	4.82	33.90
2-ethylpyridine	1.8004	7.47	17.33	1.496	5.49	8.33	–34.07
dibenzylamine	0.6908	11.65	16.39	1.5745	2.18	3.446	–36.76
1-nitrooctane	4.3559	10.42	15.57	1.433	16.73	11.46	46.01
2,2,2-trifluoroethanol	3.4195	6.26	21.32	1.281	40.64	27.68	46.81
tributyl phosphate	3.07[a]	16.86	13.36	1.424	8.39	8.34	0.62
2-methylpropanenitrile	4.191	6.55	18.41	1.379	25.06	24.42	2.63
1-chloroheptane	2.4471	12.04	15.10	1.425	5.68	5.521	2.96
tribromofluoromethane	0.4432	7.42	18.37	1.524	2.85	3	–5.14
butyl nitrate	3.6364	9.17	17.10	1.412	13.83	13.1	5.58
1-iodopentane	1.88[b]	7.52	16.48	1.495	5.36	5.78	–7.19
ethyl isothiocyanate	3.5992	4.77	18.85	1.511	21.17	19.6	8.02
tetrahydropyran	1.5202	7.35	17.25	1.419	5.12	5.66	–9.61
methyl pentanoate	1.7185	9.14	15.84	1.396	4.39	4.992	–12.02
1-bromooctane	2.5931	13.66	15.07	1.4518	5.74	5.096	12.54
benzoyl fluoride	4.0657	8.08	18.26	1.496	26.57	22.7	17.03
2,4-dimethylpyridine	2.383	7.24	17.69	1.501	7.75	9.6	–19.25
N,*N*-diethylformamide	4.1677	9.31	18.34	1.434	22.92	29.6	–22.58
trichloronitromethane	1.935	11.06	18.82	1.503	5.48	7.319	–25.17
ethyl nitrate	3.4269	9.67	18.91	1.388	14.15	19.7	–28.17
1-fluoropentane	1.85[b]	8.67	15.17	1.36	5.05	3.931	28.58
N,*N*-diethylacetamide	3.9253	10.66	17.35	1.44	21.54	32.1	–32.91
2-bromo-2-methylpropane	2.5419	8.45	15.79	1.4279	7.24	10.98	–34.08
isobutyl vinyl ether	1.2[b]	5.41	14.85	1.398	4.50	3.34	34.85
methyl nitrate	3.198	8.32	20.31	1.368	15.17	23.9	–36.51
AAPD							17.83

[a] Experimental value from ref 18. [b] Experimental value from ref 19.

of 7.25 % between experimental μ values and those calculated using B3LYP/6-311+G(3df,2p). A 44 compound subset of the DC training set was also used to test the sensitivity of ε values calculated from eq 1 to predicted values of μ calculated with B3LYP/6-311+G(3df,2p). This test produced an AAPD of 9.8 % for the DC when calculated values of μ were used in eq 1 versus 9.2 % when experimental values were used.

3. Predictions Using the Correlation

To test the predictive capability of the correlation, a test set of 42 polar compounds was developed from the data used by Sild and Karelson.[13] None of these compounds were in the DIPPR 801 database or used in development of the correlation. These compounds included a variety of chemical functional groups with ε values over nearly the entire domain of the correlation from 1 to 50. Table 3 lists the test set compounds, the values of the independent descriptors, and the predicted and experimental ε values. Values for δ were calculated from the definition of the solubility parameter,

$$\delta = \left(\frac{\Delta H_{\mathrm{vap}} - RT}{V}\right)^{0.5}\Bigg|_{T=298.15\ \mathrm{K}} \tag{3}$$

using the gas constant, R, and available literature values for the heat of vaporization, ΔH_{vap}, and liquid molar volume, V, at 298.15 K. Values of n were readily available in the literature, but values for A_{vdw} were calculated from Bondi group contributions,[19] consistent with the method by which the DIPPR 801 values are obtained.

Table 3 also shows the values and reference for the values of μ used. While experimental μ values have been reported in the literature for 20 of the 42 compounds, many of these values were measured at temperatures other than 298.15 K and/or in various solvents. As previously mentioned, the correlations were developed using gas-phase values and values measured in benzene at 298.15 K. Experimental μ values for 4[20,21] of the 42 compounds met these criteria and were used in evaluation of the test set data as shown in Table 3; all of the remaining μ values were gas-phase values calculated using B3LYP/6-311+G(3df,2p).

Values of ε predicted from the correlation of these 42 polar compounds produced an AAPD of 17.83 %, indicating no real degradation in results when eq 1 is used to predict, as opposed to correlate, ε. To our knowledge, the most accurate and generally applicable correlation for DC previously available in the literature is that by Sild and Karelson. As mentioned earlier, the correlations by Schweitzer and Morris[11] with 6 to 12 descriptors had errors of over 100 % for 7 % of the 497 compounds in the training set and errors of over 50 % for 23

Table 4. Comparison of Available Methods

	Sild and Karelson[13]	this work
no. of descriptors	6	4 + 9 O group contributions
training set	155	519
test set	46	42
AAPD for training set	23.34 %	17.78 %
AAPD for test set	39.33 %	17.83 %
combined AAPD	27.00 %	17.78 %

% of the compounds. While other correlations have been developed for the DC of specific families of chemicals, we compare here only correlations generally applicable to most organic compounds. Table 4 shows a comparison between the Sild and Karelson correlation and the one developed in this work. The correlation developed in this work is based on a much larger training set, but the test set is slightly smaller. The accuracy of the newly developed correlation is comparable to that obtained in tuning it to the training set data and is notably better than that reported for the Sild and Karelson correlation.

4. Conclusion

A new QSPR correlation for the DC has been developed using the dipole moment, van der Waals area, solubility parameter, and refractive index, descriptors readily available in the DIPPR 801 database. Different coefficients are to be used when the correlation is applied to either hydrocarbons or nonpolar fluids than when it is applied to polar, nonhydrocarbon fluids. DCs were accurately correlated for a set of 167 nonpolar and hydrocarbon chemicals with an average absolute error of 0.07 or an AAPD of 2.96 %. The correlation's coefficients for polar fluids were obtained by correlating values for 519 chemicals which gave an average absolute error of 2.05 or an AAPD of 17.78 %. The polar correlation was tested in prediction mode on a set of 42 chemicals not included in the training set with ε values ranging from 1 to 50. The test results showed little degradation from the correlating effectiveness with an AAPD of 17.83 %. Although more extensive testing is desirable, the availability of more experimental data is required to do so. We also believe the accuracy of the correlation is limited by the accuracy of the currently available experimental data. Further refinement of the correlation would likely require not only additional data but also a limitation on the training set data to that of the highest accuracy. This has not been done because of our objective to keep the correlation generally applicable to all organic compounds and the requisite need for an extensive database of 500 compounds or more to satisfy that objective. Nevertheless, these results suggest that the correlation can be used to predict ε values with an average uncertainty of about 18 % for polar compounds and of about 3 % for hydrocarbon and nonpolar compounds. The correlation is not intended for compounds where the predicted value is greater than 50. We have also shown that dipole moments obtained from B3LYP/6-311+G(3df,2p) calculations can be used in the correlation for ε, when experimental μ values are not available, with little decrease in accuracy of the predicted ε values.

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