# Abraham Model Correlations for Describing Solute Transfer Processes into Diethyl Carbonate

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**Abstract**

Experimental solubilities have been determined for 1-chloroanthraquinone, anthracene, biphenyl, pyrene, benzil, benzoic acid, acetylsalicylic acid, 4-*tert*-butylbenzoic acid, 3,4-dichlorobenzoic acid, 2-chloro-5-nitrobenzoic acid, 4-chloro-3-nitrobenzoic acid, 2-methoxybenzoic acid, 4-methoxybenzoic acid, 3,4-dimethoxybenzoic acid, 3,4,5-trimethoxybenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 4-methyl-3-nitrobenzoic acid, 4-nitrobenzoic acid, benzoin, salicylamide, thioxanthen-9-one, 1,4-dichloro-2-nitrobenzene and phenothiazine dissolved in diethyl carbonate at 298.15 K. Results of our experimental measurements, combined with published solubility and activity coefficient data, have been used to derive Abraham model correlations for describing solute transfer into diethyl carbonate. The derived mathematical correlations back-calculate the observed experimental data to within an overall standard deviation of 0.13 log units.

**Key Words and Phrases:**

Diethyl carbonate solvent; Solubilities of crystalline organic compounds; Abraham model correlations; Solute transfer processes

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## 1. Introduction

Organic solvents play an important role in many chemical manufacturing processes. They provide a liquid medium for the synthesis of new products, for the development of new analytical methodologies based on spectroscopic measurements and volumetric titrations, and for the extraction and isolation of phytochemicals from plant materials. Each year the chemical manufacturing sector consumes and disposes of several million tons of organic solvents that are harmful to the environment. The environmental impact is profound, and in many instances is irreversible. If not checked the environmental damage is likely to increase as the annual consumption of organic solvents is project to grow in future years to accommodate the expected population growth. Increased environmental awareness, combined public concern regarding workplace safety, have resulted in new governmental regulations regarding the utilization and subsequent disposal of toxic chemicals in industrial manufacturing processes. To address these concerns the manufacturing sector is continuously searching for safer solvent alternatives and for "solvent free" synthetic methods. Replacement of harmful organic solvents is not an easy task as very little information is available regarding the solubilizing properties of many of the potential solvent candidates.

In recent years [1-15] there has been renewed interest in performing solubility measurements for crystalline organic compounds dissolved both in organic mono-solvents and in binary solvent mixtures. The primary objective of these studies has been to identify suitable solvents for purifying medicinal and cosmetic compounds, pesticides and herbicides, and other synthesized chemical products through recrystallization. For the most part the fore-mentioned studies have been limited to only a handful of different organic mono-solvents and solvent

mixtures. Very little attention was given to extending the measured data to predict the solubility of the studied compounds in additional organic solvents.

Our solubilization studies [16-24] differ from those performed by other research groups in that we have used our experimental data to develop Abraham model correlations [25-27]:

$$\log P \text{ and } \log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}}\right) = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} \qquad (1)$$

$$\log K \text{ and } \log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}\right) = c_k + e_k \cdot \mathbf{E} + s_k \cdot \mathbf{S} + a_k \cdot \mathbf{A} + b_k \cdot \mathbf{B} + l_k \cdot \mathbf{L} \qquad (2)$$

that can be used to predict molar solute solubilities and infinite dilution activity coefficients in additional organic solvents. The Abraham solvation parameter model is based on a firm, fundamental understanding of how molecules interact in fluid solution. Each term on the right-hand side of Eqns. 1 and 2 represent a different type of molecular interaction as quantified by the product of a solute property times the complementary solvent property. Solute properties (called solute descriptors) are defined as follows: **E** corresponds to the molar refraction of the given solute in excess of that of a linear alkane having a comparable molecular size; **S** is a combination of the electrostatic polarity and polarizability of the dissolved solute; **A** and **B** quantify the respective hydrogen-bond donating and hydrogen-bond accepting abilities of the solute; **V** refers to the solute's McGowan molecular volume (calculated from atomic sizes and chemical bond numbers [28]); and **L** denotes the logarithm of the solute's measured gas-to-hexadecane partition coefficient at 298.15 K.

The complementary solvent properties ($c_p$, $e_p$, $s_p$, $a_p$, $b_p$, $v_p$, $c_k$, $e_k$, $s_k$, $a_k$, $b_k$, and $l_k$) in Eqns. 1 and 2 are obtained by curve-fitting logarithms of experimental water-to-organic solvent partition/transfer coefficients, log *P*, logarithms of experimental gas-to-organic solvent

partition/transfer coefficients, log $K$, and logarithms of molar solubility ratios, $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}})$ and $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}})$, in accordance to the Abraham model. The subscripts "org solv", "water" and "gas phase" associated with the molar solubilities indicate the phase to which the molar solubility pertains. For example $C^{sat}_{solute,org\ solv}$ and $C^{sat}_{solute,water}$ denote the molar solubility of the solute in the organic solvent and in water, respectively. The quantity $C^{gas}_{solute,gas}$ is the molar concentration of the solute in the gas phase whose numerical value is often determined as part of the solute descriptor calculations. The Abraham model is described in greater detail in several earlier publications [25, 26, 29-31]. The advantage that the Abraham model offers over solution models used by other researchers is that once an Abraham model equation coefficients have been determined for a given solvent, one can then predict the solubility and/or infinite dilution activity coefficients of more than 8,000 different compounds in the given solvent. Abraham model solute descriptors are readily available for over 8,000 organic, organometallic and inorganic compounds [32].

To date we have determined Abraham model process coefficients for several different classes of organic compounds including alkanes, alkylbenzene, chloroalkanes, perfluoroalkanes, halogenated benzenes, alkanols and alkanediols, alkyl alkanoates, dialkyl ethers, alkoxyalcohols, alkanenitriles, alkylformamides, alkylacetamides and many other miscellaneous organic solvents (dimethyl sulfoxides, aniline, acetophenone, benzonitrile, nitrobenzene, carbon disulfide, acetic acid, tributyl phosphate, propylene carbonate) [16-24, 27, 33-35]. Process equation coefficients have also been determined for binary aqueous-methanol [36] and binary aqueous-ethanol [37, 38] solvent mixtures. The aforementioned correlations provide the chemical manufacturer sector with predictive solubility and solute transfer expressions for a wide range of chemically diverse solvent

media. One solvent class that is not very well represented by our earlier studies is alkyl carbonates. We have studied only a single alkyl carbonate, namely propylene carbonate [39].

In the present communication we extend our solubilization studies to include diethyl carbonate, which is an important organic co-solvent used in lithium ion batteries [40, 41] and as an extraction solvent for the removal of carboxylic acids from aqueous solutions [42 - 44]. Organic carbonates have also been studied as possible "green" solvents in polymer membrane preparation [45]. As noted by Rasool and coworkers [45] "Organic carbonates in general are environmentally friendly, have low eco-toxicity, and show good biodegradability." Experimental solubilities have been determined for 1-chloroanthraquinone, anthracene, biphenyl, pyrene, benzil, benzoic acid, acetylsalicylic acid, 4-*tert*-butylbenzoic acid, 3,4-dichlorobenzoic acid, 2-chloro-5-nitrobenzoic acid, 4-chloro-3-nitrobenzoic acid, 2-methoxybenzoic acid, 4-methoxybenzoic acid, 3,4-dimethoxybenzoic acid, 3,4,5-trimethoxybenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 4-methyl-3-nitrobenzoic acid, 4-nitrobenzoic acid, benzoin, salicylamide, thioxanthen-9-one, 1,4-dichloro-2-nitrobenzene and phenothiazine dissolved in diethyl carbonate at 298.15 K. Results of our measurements, combined with published solubility data for helium [46], neon [46], argon [46], krypton [46], xenon [46], hydrogen [46], nitrogen [46], oxygen [47], sulfur hexafluoride [46], carbon dioxide [48], tetrafluorocarbon [46], hydrogen sulfide [48], methane [46], ethane [46], ethene [46], 1,1,1,2-tetrafluoroethane [49] and diphenyl carbonate [50] and published infinite dilution activity coefficient data for hexane [51], octane [52], dodecane [53], cyclohexane [54], benzene [55], carbon tetrachloride [56], methyl *tert*-butyl ether [57] and dimethyl carbonate [58, 59], have been used to derive Abraham model correlations for solute transfer into diethyl carbonate from both water (Eqn. 1) and from the gas phase (Eqn. 2).

## 2. Chemical Materials and Experimental Methodology

In assembling the crystalline organic compounds for the solubility determinations we selected compounds that exhibit a wide range of chemical diversity and that span a wide range of solute descriptors values. All chemicals used in the solubility measurements were purchased from commercial sources. The sample of diethyl carbonate was dried over activated molecular sieves and distilled shortly before use. Samples of 1-chloroanthraquinone, benzil, salicylamide, thioxanthen-9-one, pyrene, 1,4-dichloro-2-nitrobenzene, and biphenyl were recrystallized three times from anhydrous methanol and dried for two days at 333 K prior to use. Anthracene was recrystallized three times from anhydrous acetone and dried for two days at 333 K. The carboxylic acid solutes were dried for two days at 333 K prior to use. Gas chromatographic analysis (flame ionization detector) indicated that the purities of purified samples of diethyl carbonate, 1-chloroanthraquinone, benzil, anthracene, biphenyl, pyrene, 1,4-dichloro-2-nitrobenzene, thioxanthen-9-one and salicylamide were 0.997 mass fraction. The purities of the fourteen carboxylic acid samples were determined by a non-aqueous titrimetric method based on the published method of Fritz and Lisicki [60]. The method was modified for health reasons in that benzene was replaced by toluene in preparing the titration solvent. Acid-base titrations with freshly standardized sodium methoxide (thymol blue indicator) indicated that the purities of acetylsalicylic acid, benzoic acid, 4-*tert*-butylbenzoic acid, 3,4-dichlorobenzoic acid, 2-chloro-5-nitrobenzoic acid, 4-chloro-3-nitrobenzoic acid, 2-methoxybenzoic acid, 4-methoxybenzoic acid, 3,4-dimethoxybenzoic acid, 3,4,5-trimethoxybenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 4-methyl-3-nitrobenzoic acid, and 4-nitrobenzoic acid were 0.998 (±0.003) mass fraction. The commercial suppliers and chemical purities of the chemicals used in the solubility measurements are summarized in Table 1.

Table 1. Chemical Sources and Mass Fraction Purities of Chemicals Used in the Solubility Studies

| Chemical | Supplier | Purification Method | Purity (Mass Fraction) |
|---|---|---|---|
| | | | |
| Diethyl carbonate | Acros Organics, Morris Plains, New Jersey, USA | Stored over molecular and distilled | 0.997 |
| 1-Chloroanthraquinone | Aldrich Chemical Company, Milwaukee, Wisconsin, USA | Recrystallization from anhydrous methanol | 0.997 |
| Phenothiazine | Acros Organics | Used as received | 0.99 |
| Biphenyl | Aldrich Chemical Company | Recrystallization from anhydrous methanol | 0.997 |
| Benzil | Aldrich Chemical Company | Recrystallization from anhydrous methanol | 0.997 |
| Anthracene | Aldrich Chemical Company | Recrystallization from anhydrous acetone | 0.997 |
| Pyrene | Aldrich Chemical Company | Recrystallization from anhydrous methanol | 0.997 |
| Acetylsalicylic acid | Aldrich Chemical Company | Dried for two days at 333 K | 0..998 |
| Thioxanthen-9-one | Aldrich Chemical Company | Recrystallization from anhydrous methanol | 0.997 |
| Salicylamide | Aldrich Chemical Company | Recrystallization from anhydrous methanol | 0.997 |
| Benzoin | Aldrich Chemical Company | Recrystallization from anhydrous methanol | 0.997 |
| 1,4-Dichloro-2-nitrobenzene | TCI America Chemical Company, Portland, Oregon, USA | Recrystallization from anhydrous methanol | 0.997 |
| Benzoic acid | Aldrich Chemical Company | Dried for two days at 333 K | 0.998 |
| 4-*tert*-Butylbenzoic acid | TCI America Chemical Company | Dried for two days at 333 K | 0.998 |
| 2-Chloro-5-nitrobenzoic acid | Acros Organics | Dried for two days at 333 K | 0.998 |
| 4-Chloro-3-nitrobenzoic acid | Acros Organics | Dried for two days at 333 K | 0.998 |
| 3,4-Dichlorobenzoic acid | Aldrich Chemical Company | Dried for two days at 333 K | 0.998 |
| 2-Methoxybenzoic acid | Aldrich Chemical Company | Dried for two days at 333 K | 0.998 |
| 4-Methoxybenzoic acid | Aldrich Chemical Company | Dried for two days at 333 K | 0.998 |

| | | | |
|---|---|---|---|
| 3,4-Dimethoxybenzoic acid | Across Organics | Dried for two days at 333 K | 0.998 |
| 3,4,5-Trimethoxybenzoic acid | Aldrich Chemical Company | Dried for two days at 333 K | 0.998 |
| 2-Methylbenzoic acid | Aldrich Chemical Company | Dried for two days at 333 K | 0.998 |
| 3-Methylbenzoic acid | Aldrich Chemical Company | Dried for two days at 333 K | 0.998 |
| 4-Methyl-3-nitrobenzoic acid | Aldrich Chemical Company | Dried for two days at 333 K | 0.998 |
| 4-Nitrobenzoic acid | Acros Organics | Dried for two days at 333 K | 0.998 |
| Toluene | Aldrich Chemical Company | None | 0.998, anhydrous |
| Sodium methoxide, 25 mass % solution in methanol | Aldrich Chemical Company | None | |
| 2-Propanol | Aldrich Chemical Company | None | 0.99 |

Solubilities of the 24 crystalline organic compounds were measured using a static equilibration method followed by a spectroscopic determination of the concentration of the dissolved solute in the saturated solution based on the Beer-Lambert law. The experimental methodology that we use has been given in many of our earlier publications [61-65], and to conserve journal space will only be briefly described in this communication. Aliquots of the saturated solutions were transferred by syringe into weighed volumetric flasks after the samples had equilibrated in sealed amber glass bottles in a constant temperature water bath at 298.15 ± 0.05 K for at least three days. The samples were periodically agitated to facilitate dissolution and mixing. The volumetric flasks containing the transferred aliquots were weighed on an electronic analytical balance. The transferred solutions were diluted quantitatively with 2-propanol. Absorbances of the diluted solutions and of the nine standard solutions of known solute concentrations were recorded on a Milton Roy Spectronic 1000 Plus spectrophotometer (Milton Roy, Rochester, NY, USA). The concentration of each diluted solution was computed from a

Beer-Lambert law plot of absorbance versus concentration curve obtained from the measured absorbances of nine standard solutions of known solute molarity. The analysis wavelengths and concentration ranges used for each solute have been given in our earlier publications [61-81]. We checked to make sure that diethyl carbonate did not absorb light at the analysis wavelengths and at the diethyl carbonate concentrations in the diluted solutions.

Molar concentrations of the diluted samples deduced from the Beer-Law law graph were converted into mole fraction solubilities using the volume of the volumetric flasks that the solute was transferred into, the mass of the sample analyzed, molar masses of the solvent and the respective solutes, and any dilutions that may have been needed in order for the sample's measured absorbance to fall on the Beer-Lambert law curve. We checked each equilibrated solid phase for possible solvate formation by determining the melting point temperature of the equilibrated solid phases recovered from the saturated solutions after the solubility measurements of each solute were completed. The melting point temperature of each equilibrated solid phase was within ± 0.5 K of the melting point temperature of the commercial sample or recrystallized compound prior to being in contact with the diethyl carbonate solvent.

The experimental mole fraction solubilities, $x_{solute}^{sat}$, of the crystalline organic solutes in diethyl carbonate are tabulated in the second column of Table 2. The numerical values represent the average of 4 to 10 independent experimental determinations, which were reproducible to within ± 2 % (relative error). To the best of our knowledge there are no published solubility data for these organic solutes in diethyl carbonate that we can compare our experimental values against. The only published solubility data that we were able to find for solid organic compounds dissolved in diethyl carbonate were the value previously published by Li and coworkers [50] for diphenyl carbonate.

Table 2. Mole Fraction Solubilities, $x_{solute}^{sat}$, of 24 Crystalline Organic Compounds Dissolved in Diethyl Carbonate at a Temperature of 298.15 K

| Crystalline Organic Compound | $x_{solute}^{sat}$ |
|---|---|
| | |
| 1-Chloroanthraquinone | 0.00775 |
| Phenothiazine | 0.0376 |
| Biphenyl | 0.234 |
| Benzil | 0.133 |
| Anthracene | 0.00547 |
| Pyrene | 0.0451 |
| Acetylsalicylic acid | 0.0226 |
| Thioxanthen-9-one | 0.00323 |
| Salicylamide | 0.0364 |
| Benzoin | 0.109 |
| 1,4-Dichloro-2-nitrobenzene | 0.438 |
| Benzoic acid | 0.112 |
| 4-*tert*-Butylbenzoic acid | 0.0332 |
| 2-Chloro-5-nitrobenzoic acid | 0.0309 |
| 4-Chloro-3-nitrobenzoic acid | 0.0133 |
| 3,4-Dichlorobenzoic acid | 0.00809 |
| 2-Methoxybenzoic acid | 0.0366 |
| 4-Methoxybenzoic acid | 0.00600 |
| 3,4-Dimethoxybenzoic acid | 0.00401 |
| 3,4,5-Trimethoxybenzoic acid | 0.00698 |
| 2-Methylbenzoic acid | 0.0996 |
| 3-Methylbenzoic acid | 0.0951 |
| 4-Methyl-3-nitrobenzoic acid | 0.0123 |
| 4-Nitrobenzoic acid | 0.00614 |

## 3. Development of Abraham Model Correlations for Solute Transfer into Diethyl Carbonate

Development of Abraham model correlations to describe solute transfer into diethyl carbonate requires constructing an Eqn 1 and Eqn. 2 for each of the 50 individual organic and inorganic solutes considered in the current study. The solute descriptors needed for the right-hand

sides of the two equations are tabulated in Table 3. The transfer properties needed on the left-hand side of Eqns. 1 and 2 are calculated from the experimental mole fraction solubility data given in Table 2 or from the experimental solubility data and activity coefficients retrieved from the published chemical and engineering. Mole fraction based solubilities are converted into molar solubilities by dividing $x_{solute}^{sat}$ by the ideal molar volume of the saturated solution:

$$C_{solute,org\ solv}^{sat} = \frac{x_{solute}^{sat}}{(1-x_{solute}^{sat})\,V_{solvent} + x_{solute}^{sat}\,V_{solute}} \quad (3)$$

The numerical values used for the molar volumes of the hypothetical subcooled liquid solutes are given in our earlier publications [63-86], along with the aqueous molar solubilities, $C_{solute,water}^{sat}$, and solute molar gas concentrations, $C_{solute,gas}^{gas}$, needed in calculating the two molar solubility ratios. The mole fraction solubility of diphenyl carbonate in diethyl carbonate that was retrieved from the published literature [50] was similarly converted to a molar solubility. The molar solubility ratios are tabulated in the eighth and ninth columns of Table 3.

Table 3. Logarithms of Experimental Partition Coefficients, log *P* and log *K*, Logarithms of Molar Solubility Ratios, $\log(\frac{C_{solute,org\ solv}^{sat}}{C_{solute,water}^{sat}})$ and $\log(\frac{C_{solute,org\ solv}^{sat}}{C_{solute,gas\ phase}^{sat}})$, and Solute Descriptors for Organic Compounds and Inorganic Gases Dissolved in Diethyl Carbonate at 298.15 K

| Solute | **E** | **S** | **A** | **B** | **L** | **V** | Log *K*[a] | Log *P*[b] | Ref. |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | |
| Helium | 0.000 | 0.000 | 0.000 | 0.000 | -1.741 | 0.0680 | -1.504 | 0.516 | [46] |
| Neon | 0.000 | 0.000 | 0.000 | 0.000 | -1.575 | 0.0850 | -1.378 | 0.582 | [46] |
| Argon | 0.000 | 0.000 | 0.000 | 0.000 | -0.688 | 0.1900 | -0.571 | 0.899 | [46] |
| Krypton | 0.000 | 0.000 | 0.000 | 0.000 | -0.211 | 0.2460 | -0.132 | 1.078 | [46] |
| Xenon | 0.000 | 0.000 | 0.000 | 0.000 | 0.378 | 0.3290 | 0.420 | 1.390 | [46] |
| Hydrogen | 0.000 | 0.000 | 0.000 | 0.000 | -1.200 | 0.1086 | -1.107 | 0.613 | [46] |
| Nitrogen | 0.000 | 0.000 | 0.000 | 0.000 | -0.978 | 0.2222 | -0.813 | 0.987 | [46] |
| Oxygen | 0.000 | 0.000 | 0.000 | 0.000 | -0.723 | 0.1830 | -0.713 | 0.787 | [47] |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Sulfur hexafluoride | -0.600 | -0.200 | 0.000 | 0.000 | -0.120 | 0.4643 | 0.018 | 2.238 | [46] |
| Tetrafluoromethane | -0.580 | -0.260 | 0.000 | 0.000 | -0.817 | 0.3203 | -0.667 | 1.623 | [46] |
| Carbon dioxide | 0.000 | 0.280 | 0.050 | 0.100 | 0.058 | 0.2809 | 0.713 | 0.793 | [48] |
| Hydrogen sulfide | 0.350 | 0.310 | 0.100 | 0.070 | 0.723 | 0.2721 | 1.056 | 0.656 | [48] |
| Methane | 0.000 | 0.000 | 0.000 | 0.000 | -0.323 | 0.2495 | -0.261 | 1.199 | [46] |
| Ethane | 0.000 | 0.000 | 0.000 | 0.000 | 0.492 | 0.3904 | 0.495 | 1.835 | [46] |
| Ethene | 0.107 | 0.100 | 0.000 | 0.070 | 0.289 | 0.3474 | 0.499 | 1.439 | [46] |
| Hexane | 0.000 | 0.000 | 0.000 | 0.000 | 2.668 | 0.9540 | 2.887 | 4.707 | [51] |
| Octane | 0.000 | 0.000 | 0.000 | 0.000 | 3.677 | 1.2358 | 3.437 | 5.547 | [52] |
| Dodecane | 0.000 | 0.000 | 0.000 | 0.000 | 5.696 | 1.7994 | 5.441 | 7.971 | [53] |
| Cyclohexane | 0.305 | 0.100 | 0.000 | 0.000 | 2.964 | 0.8454 | 2.610 | 3.510 | [54] |
| 1,1,1,2-Tetrafluoroethane | -0.410 | 0.410 | 0.060 | 0.020 | 0.530 | 0.4612 | 1.562 | 1.972 | [49] |
| Tetrachloromethane | 0.460 | 0.380 | 0.000 | 0.000 | 2.823 | 0.7391 | 3.134 | 3.194 | [56] |
| Benzene | 0.610 | 0.520 | 0.000 | 0.140 | 2.786 | 0.7164 | 3.232 | 2.602 | [55] |
| Methyl *tert*-butyl ether | 0.024 | 0.220 | 0.000 | 0.590 | 2.380 | 0.8718 | 2.674 | 1.084 | [57] |
| Dimethyl carbonate | 0.142 | 0.540 | 0.000 | 0.570 | 2.328 | 0.6644 | 3.308 | | [58,59] |
| Diethyl carbonate | 0.060 | 0.580 | 0.000 | 0.530 | 3.412 | 0.9462 | 4.099 | 1.659 | Unity |
| Diphenyl carbonate | 1.280 | 1.530 | 0.000 | 0.590 | 7.843 | 1.5982 | 9.374 | 4.242 | [50] |
| 1-Chloroanthraquinone | 1.900 | 1.790 | 0.000 | 0.570 | 9.171 | 1.6512 | 10.376 | 4.342 | This work |
| Anthracene | 2.290 | 1.340 | 0.000 | 0.280 | 7.568 | 1.4544 | 8.111 | 5.081 | This work |
| Biphenyl | 1.360 | 0.990 | 0.000 | 0.260 | 6.014 | 1.3242 | 6.540 | 4.590 | This work |
| Pyrene | 2.808 | 1.710 | 0.000 | 0.280 | 8.833 | 1.5850 | 9.211 | 5.711 | This work |
| Benzil | 1.445 | 1.590 | 0.000 | 0.620 | 7.611 | 1.6374 | 8.930 | 4.060 | This work |
| Benzoic acid | 0.730 | 0.900 | 0.590 | 0.400 | 4.657 | 0.9317 | 6.660 | 1.520 | This work |
| Acetylsalicylic acid | 0.781 | 1.690 | 0.710 | 0.670 | 6.279 | 1.2879 | 9.446 | 0.946 | This work |
| 4-tert-Butylbenzoic acid | 0.730 | 1.111 | 0.551 | 0.443 | 6.547 | 1.4953 | 8.553 | 3.329 | This work |
| 3,4-Dichlorobenzoic acid | 0.950 | 0.920 | 0.670 | 0.260 | 5.623 | 1.1766 | 7.542 | 2.802 | This work |
| 2-Chloro-5-nitrobenzoic acid | 1.250 | 1.400 | 0.670 | 0.460 | 6.513 | 1.2283 | 8.941 | 1.991 | This work |
| 4-Chloro-3-nitrobenzoic acid | 1.250 | 1.470 | 0.700 | 0.440 | 6.685 | 1.2283 | 9.249 | 2.039 | This work |
| 2-Methoxybenzoic acid | 0.899 | 1.410 | 0.450 | 0.620 | 5.636 | 1.1313 | 7.831 | 1.031 | This work |
| 4-Methoxybenzoic acid | 0.899 | 1.250 | 0.620 | 0.520 | 5.741 | 1.1313 | 8.192 | 1.492 | This work |
| 3,4-Dimethoxybenzoic acid | 0.950 | 1.646 | 0.570 | 0.755 | 6.746 | 1.3309 | 9.459 | 1.012 | This work |
| 3,4,5-Trimethoxybenzoic acid | 1.001 | 1.760 | 0.603 | 0.850 | 7.711 | 1.5309 | 10.562 | 1.307 | This work |
| 2-Methylbenzoic acid | 0.730 | 0.840 | 0.420 | 0.440 | 4.677 | 1.0726 | 6.272 | 1.972 | This work |
| 3-Methylbenzoic acid | 0.730 | 0.890 | 0.600 | 0.400 | 4.819 | 1.0726 | 7.012 | 2.032 | This work |
| 4-Methyl-3-nitrobenzoic acid | 1.040 | 1.461 | 0.659 | 0.521 | 6.434 | 1.2468 | 8.972 | 1.687 | This work |
| 4-Nitrobenzoic acid | 0.990 | 1.520 | 0.680 | 0.400 | 5.770 | 1.1059 | 8.582 | 1.682 | This work |
| Thioxanthen-9-one | 1.940 | 1.441 | 0.000 | 0.557 | 8.436 | 1.5357 | 9.031 | 3.963 | This work |
| Benzoin | 1.585 | 2.115 | 0.196 | 0.841 | 9.159 | 1.6804 | 11.351 | 2.620 | This work |
| Salicylamide | 1.160 | 1.650 | 0.630 | 0.480 | 5.910 | 1.0315 | 8.912 | 1.227 | This work |
| 1,4-Dichloro-2-nitrobenzene | 1.120 | 1.289 | 0.000 | 0.199 | 5.783 | 1.1354 | 6.747 | 3.846 | This work |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Phenothiazine | 1.890 | 1.560 | 0.310 | 0.300 | 8.389 | 1.4789 | 9.987 | 4.584 | This work |
| | | | | | | | | | |

[a] For crystalline solutes the tabulated value is $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}})$.

[b] For crystalline solutes the tabulated value is $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}})$.

The experimental data for the dissolved liquid solutes was given in the published literature as the infinite dilution activity coefficient, $\gamma^{\infty}_{solute}$. Infinite dilution activity coefficients are converted to the logarithm of the gas-to-organic solvent partition coefficients through standard thermodynamic relationships:

$$\log K = \log(\frac{RT}{\gamma^{\infty}_{solute}\, p^{o}_{solute}\, V_{solvent}}) \quad (4)$$

where $R$ is the universal gas constant and $p^{o}_{solute}$ is the saturated vapor pressure of a pure solute at the solution temperature, which in this study is $T$ = 298.15 K. As an informational note infinite dilution activity coefficient of diethyl carbonate dissolved in itself is unity.

The published solubility data for the gaseous solutes was given either in terms of gas-to-diethyl carbonate partition coefficient, $K$, or in terms of the Henrys law constant, $K_{\text{Henry}}$. Henrys law constants are converted to log $K$ values through Eqn. 5.

$$\log K = \log(\frac{RT}{K_{Henry}\, V_{solvent}}) \quad (5)$$

The log $K$ values for the liquid and gaseous solutes are converted to log $P$ values by:

$$\log P = \log K - \log K_{\text{water}} \quad (6)$$

where $K_{\text{water}}$ is the solute's gas-to-water partition coefficient, which is available for the different solutes considered in the current study [82-86]. We have also tabulated the numerical values of log $K$ and log $P$ values for the liquid and gases in the eighth and ninth columns of Table 3. As the

column headings indicate the tabulated numerical values for the crystalline organic solutes pertain to the two respective solubility ratios, $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}})$ and $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}})$.

Our experimental measurements, combined with our search of the published literature, have experimental partition coefficients and solubility ratios for 50 different organic and inorganic compounds. The solutes are chemically diverse, they cover a wide range of solute polarities and hydrogen-bonding capability, and include several fairly strong H-bond donors (acetylsalicylic acid, **A** = 0.710; 4-chloro-3-nitrobenzoic acid, **A** = 0.700) and several fairly strong H-bond acceptors (3,4,5-trimethoxybenzoic acid, **B** = 0.850; benzoin, **B** = 0.841). Regression analysis of the experimental values yielded the following two Abraham model expressions:

$$\log P \text{ and } \log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}}) = 0.133(0.044) + 0.135(0.075)\ \mathbf{E} - 0.309(0.121)\ \mathbf{S} - 1.532(0.103)\ \mathbf{A} - 4.816(0.183)\ \mathbf{B} + 4.398(0.069)\ \mathbf{V} \quad (7)$$

(with N = 49, SD = 0.134, $R^2$ = 0.994, F = 1333)

$$\log K \text{ and } \log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}) = 0.092(0.027) - 0.598(0.057)\ \mathbf{E} + 1.527(0.078)\ \mathbf{S} + 1.942(0.088)\ \mathbf{A} + 0.948(0.014)\ \mathbf{L} \quad (8)$$

(with N = 50, SD = 0.117, $R^2$ = 0.999, F = 13898)

The correlations were obtained using the IBM SPSS Statistical 22 commercial software. The statistical information pertaining to each correlation is given below the respective correlation, where N refers to the number of experimental data points used in determining the equation coefficients, SD is the standard deviation, $R^2$ corresponds to the squared correlation coefficient, and F represents the Fisher F-statistic. Standard errors in the equation coefficients (at 95 % level) are given in parenthesis after the coefficient itself. As an informational note the $b_k \cdot \mathbf{B}$ was

removed from Eqn. 8 because diethyl carbonate lacks an acidic hydrogen and therefore cannot act as a hydrogen-bond donor. Removal of the $b_k \cdot \mathbf{B}$ led to an insignificant increase in the standard deviation, from SD = 0.115 to SD = 0.117. The $b_p \cdot \mathbf{B}$ term was retained in Eqn. 7, however, as the expression pertains to solute transfer into diethyl carbonate from water. Here the $b_p$ equation coefficient represents the difference in the acidity of diethyl carbonate and water, which does possess two acidic hydrogens capable of engagement in hydrogen-bond formation.

As noted in the introduction a major advantage that the Abraham model offers over the solution models that other research groups are using to mathematically describe experimental solubility data is that the derived correlations can be used to predict the solubility and/or infinite dilution activity coefficient of many additional organic, organometallic and inorganic solutes dissolved in the given solvent media. An indication of Eqns. 7 and 8 ability to estimate partition coefficients and solubility ratios can be obtained by examining each correlation's ability to describe the 50 experimental values given in Table 3. The small standard deviations, SD = 0.134 log units and SD = 0.117 log units, and near unity squared correlation coefficients, $R^2 = 0.994$ and $R^2 = 0.999$, indicate that Eqs. 7 and 8 provide reasonably accurate mathematical descriptions of the observed experimental data used in both regression analyses. Figures 1 and 2 provide a graphical comparison of the experimental data versus back-calculated values based on Eqs. 7 and 8, respectively. As an informational note the experimental log *K* and $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}})$ data span a range of just under 12 log units, from log *K* = -1.504 for helium to $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}) = 11.351$ for benzoin. A slightly smaller range of approximately 7.5 log units is covered by the experimental log *P* and $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}})$ data.

Diethyl carbonate is the second carbonate solvent that we have studied. Previously we determined Abraham model correlations for propylene carbonate [39]:

$$\log P \text{ and } \log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}}\right) = 0.004 + 0.168\ \mathbf{E} + 0.504\ \mathbf{S} - 1.283\ \mathbf{A} - 4.407\ \mathbf{B} + 3.421\ \mathbf{V} \quad (9)$$

$$\log K \text{ and } \log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}\right) = -0.356 - 0.413\ \mathbf{E} + 2.587\ \mathbf{S} + 2.207\ \mathbf{A} + 0.455\ \mathrm{B} + 0.717\ \mathbf{L} \quad (10)$$

based on experimental solubility and activity coefficient data for 69 compounds. The equation coefficients of the two carbonate solvents are somewhat different. Propylene carbonate exhibits greater dipolarity/polarizability, and is a better H-bond acceptor and H-bond donor as evidenced by the larger $s_k$, $b_k$ and $a_k$ equation coefficients.

## 4. Conclusion

Mathematical expressions based on the Abraham solvation parameter model have been shown to provide reasonably accurate correlations of the solute transfer properties of a wide range of organic and inorganic compounds into diethyl carbonate from both water and from the gas phase. Experimental properties that were described by the derived Abraham model expressions include the logarithm of the water-to-diethyl carbonate transfer coefficient, the logarithm of the gas-to-diethyl carbonate transfer coefficient, and the logarithms of two molar solubility ratios given by $\log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}}\right)$, $\log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}\right)$. The derived correlations described the fore-mentioned experimental solute transfer properties to within 0.13 log units (or less). Based on our more than 20 years of experience in using the Abraham model we believe that our derived Eqns. 7 and 8 will provide reasonably accurate predictions of the log *P*, log *K*, $\log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}}\right)$ and

$\log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}\right)$ values for additional organic and inorganic compounds dissolved in diethyl carbonate at 298.15 K, provided of course that the solute descriptors of the compounds fall within the range of numerical values used in obtaining these correlations. Partition coefficients predicted by the Abraham model can be transformed into $\gamma^{\infty}_{solute}$ values through Eqs. 4 and 6. In closing we note that predicted log *P* and log *K* values at 298.15 K can be extrapolated to slightly lower and higher temperatures using our published enthalpy of solvation correlations, $\Delta H_{solv}$, [87] based on experimental $\Delta H_{solv}$ data for 80 solutes dissolved in diethyl carbonate. Our published Abraham model correlations provide the manufacturing sector with important tools to aid in the solvent selection process.

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**Disclosure statement**

No potential conflict of interest was reported by the authors.

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Figure 1

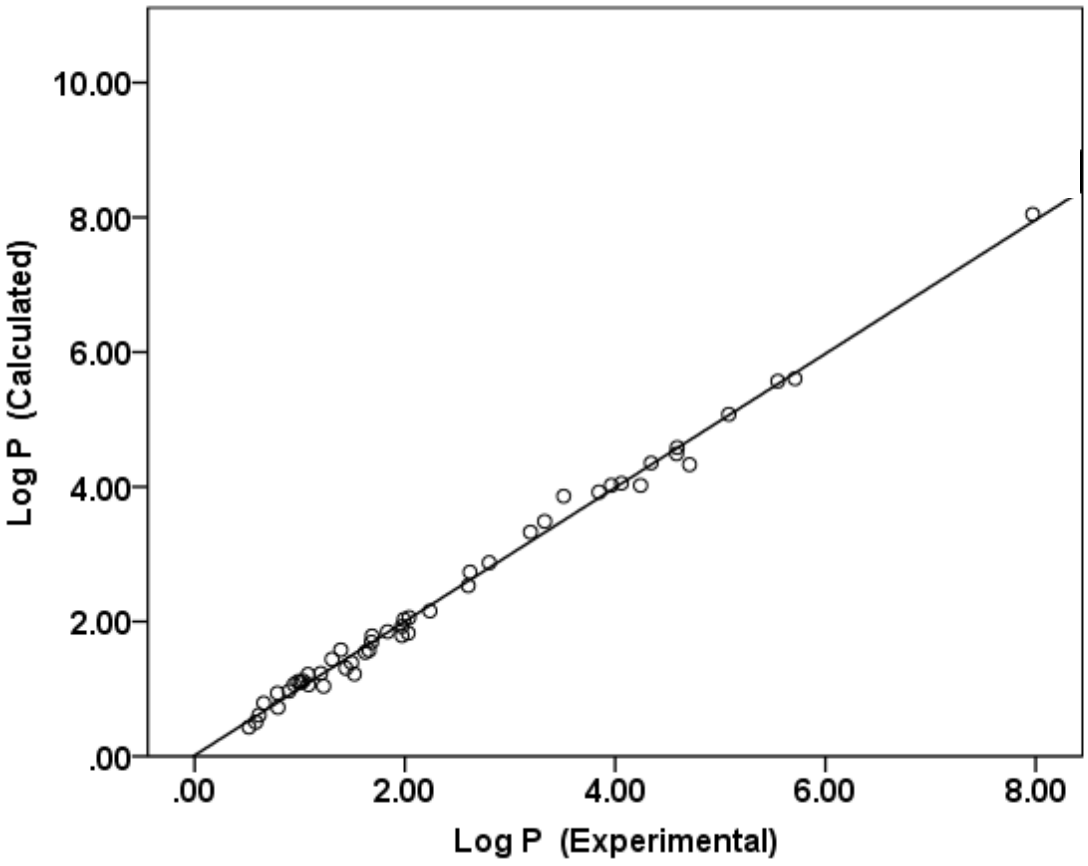


Figure 1. Comparison between the experimental log *P* and $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}})$ data and back-calculated values based on Eq. 7.

Figure 2

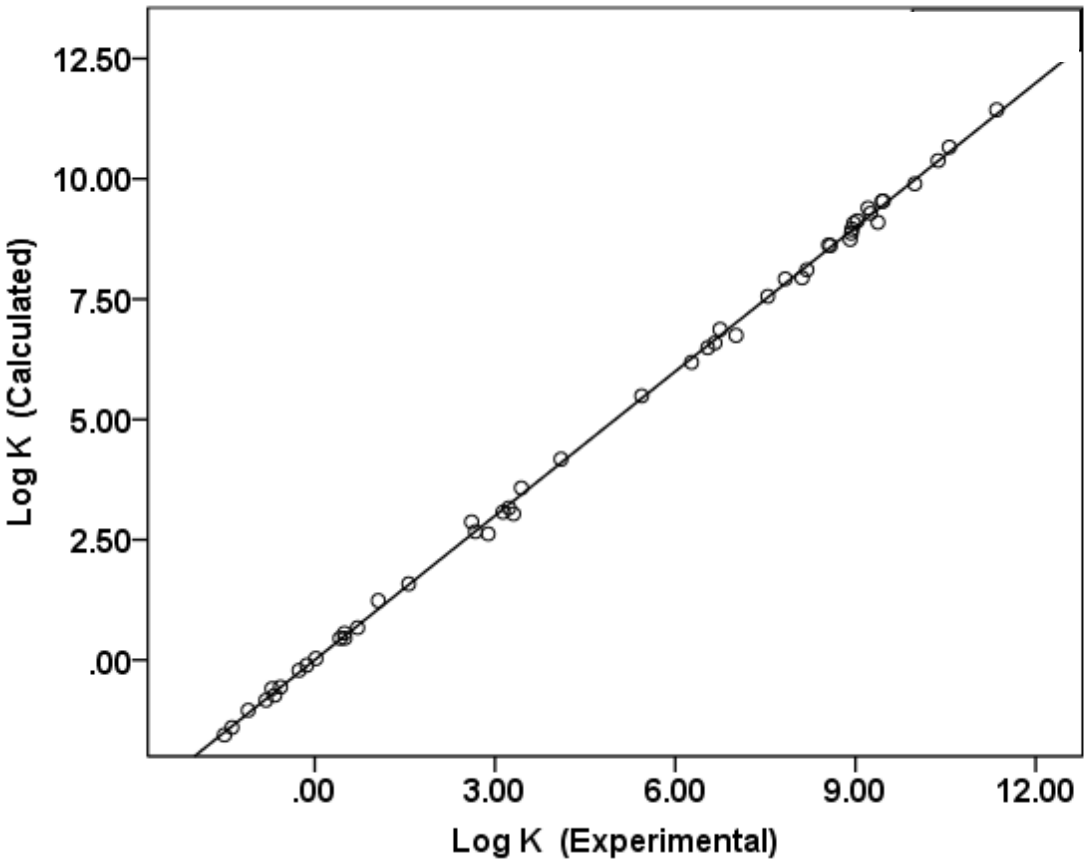


Figure 2. Comparison between the experimental log $K$ and $\log(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}})$ data and back-calculated values based on Eq. 8.