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Development of Abraham Model Correlations for Solute Transfer into the *tert*-Butyl Acetate Mono-Solvent and Updated Equations for Both Ethyl Acetate and Butyl Acetate

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Abstract: Experimental solubilities were determined for 31 solid nonelectrolyte organic compounds dissolved in *tert*-butyl acetate at 298.15 K. Results of the experimental measurements were combined with published mole fraction solubility data for two lipid-lowering medicinal compounds (lovastatin and simvastatin) in order to derive Abraham model expressions for solute transfer into the *tert*-butyl acetate mono-solvent. The derived correlations provided an accurate mathematical description of the observed experimental data. As part of the current study, previously published Abraham model solvent correlations for both ethyl acetate and butyl acetate were updated using much larger datasets that contained an additional 64 and 35 experimental data points, respectively. The mathematical correlations presented in the current study describe the observed solubility ratios of solutes dissolved in *tert*-butyl acetate, ethyl acetate, and butyl acetate to within an overall standard deviation of 0.15 log units or less.

Keywords: Abraham model correlations; molar solubility ratios; *tert*-Butyl acetate solvent; ethyl acetate; butyl acetate solvent

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1. Introduction

Individuals employed by the chemical manufacturing sector handle and are exposed to organic solvents on a daily basis. Organic solvents serve as the solubilizing reaction media in the preparation of new chemical products, as cleansing and degreasing agents for chemical glassware and industrial machinery, as components of aqueous–organic biphasic extraction systems used in the removal of unwanted impurities from synthesized chemical materials, and as dispersing agents in paint and cosmetic products. Organic solvents have also been used to extract biochemical materials from plants and to preconcentrate and remove trace organic analytes from chemical samples prior to gas–liquid and high-performance chromatographic analyses. Several million tons of petroleum-based organic solvents are purchased and discarded on an annual basis. Governmental regulations pertaining to chemical waste disposal have encouraged the manufacturing sector to utilize more environmentally compatible organic solvents, to search for solvent-free synthetic processes, and to design effective solvent recovery methods in order to reduce the quantity of hazardous materials that are released into the natural environment.

Replacing hazardous organic solvents with safer chemical alternatives is not an easy task. Industrial processes are often designed around the specific solvent that is currently being used. Altering an existing process can be an expensive endeavor, even if one has identified a safer solvent which possesses suitable physical and chemical properties. Our contribution in the solvent selection and replacement process has been to develop mathematical Abraham model expressions [1–4] that enable process design engineers to predict molar solubilities of chemical reactants, synthesized chemical products, and reaction by-products in a wide range of organic solvents of varying polarity and hydrogen-bonding

character. Unlike physical properties such as density, viscosity, and vapor pressure, one cannot easily locate needed solubility data in the published chemical and engineering literature. Solubility data is solute-solvent specific in nature, and it is not feasible to determine solubilities for every possible combination of chemical compounds. Currently there are more than 60 million known chemical compounds [5], and the number continually increases with each newly synthesized organic/inorganic molecule.

The Abraham model is among the simplest and most versatile predictive solubility expressions that have been developed in the past 30 years. The basic model [6–9] describes solute transfer, which, in the current study, is given by the logarithm of molar solubility ratios, log ($C_{S,organic}/C_{S,water}$), and log ($C_{S,organic}/C_{S,gas}$), in terms of:

$$\log (C_{S,organic}/C_{S,water}) = e_{eq\,1} \times \mathbf{E} + s_{eq\,1} \times \mathbf{S} + a_{eq\,1} \times \mathbf{A} + b_{eq\,1} \times \mathbf{B} + v_{eq\,1} \times \mathbf{V} + c_{eq\,1} \quad (1)$$

$$\log (C_{S,organic}/C_{S,gas}) = e_{eq\,2} \times \mathbf{E} + s_{eq\,2} \times \mathbf{S} + a_{eq\,2} \times \mathbf{A} + b_{eq\,2} \times \mathbf{B} + l_{eq\,2} \times \mathbf{L} + c_{eq\,2} \quad (2)$$

the molecular solute–solvent interactions that govern the dissolution process. The subscripts "organic", "water", and "gas" on solubility ratios denote the phase to which the molar solute concentration pertains. Each molecular interaction is quantified as the product of a solute property multiplied by the complimentary solvent property. Solute properties (also called solute descriptors) are denoted by the capitalized alphabetical characters on the right-hand side of Equations (1) and (2) and are defined as follows: **A** and **B** refer to the respective overall hydrogen-bond donating and accepting capacities of the dissolved solute; **E** corresponds the molar refraction of the given solute (in units of (cm^3 mol^{-1})/10) in excess of that of a linear alkane having a comparable molecular size; **L** is the logarithm of the solute's gas-to-hexadecane partition coefficient determined at 298.15 K; **S** represents a combination of the electrostatic polarity and polarizability of the solute; **V** denotes the McGowan molecular volume of the solute (in units of (cm^3 mol^{-1})/100) calculated from atomic sizes and chemical bond numbers. The complimentary solvent properties in Equations (1) and (2) are given by the lowercase alphabetical characters ($c_{eq\,1}$, $e_{eq\,1}$, $s_{eq\,1}$, $a_{eq\,1}$, $b_{eq\,1}$, $v_{eq\,1}$, $c_{eq\,2}$, $e_{eq\,2}$, $s_{eq\,2}$, $a_{eq\,2}$, $b_{eq\,2}$, and $l_{eq\,2}$). Numerical values of the solvent properties are determined by regressing measured molar solubility ratio data in accordance with Equations (1) and (2). Once determined, the lowercase alphabetical characters allow one to predict the molar solubilities of additional solutes in the given organic solvent, provided, of course, that the solute descriptors are known. Currently, equation coefficients are known for slightly more than 130 different organic solvents and binary aqueous-organic solvent mixtures [10]. This represents only a small fraction of the organic solvents currently used in industrial manufacturing processes and consumer product formulations. Less than half of the solvents for which equation coefficients have been obtained fall into the classification of "preferred" and/or "recommended" on the solvent selection guide developed by pharmaceutical companies [11–13].

In the current study, we extend our earlier considerations to include the *tert*-butyl acetate mono-solvent, which is on the list of "recommended" organic solvents [14], along with several other alkyl acetates like ethyl acetate, propyl acetate, isopropyl acetate, and butyl acetate [11,15–17]. Alkyl acetates and other esters score well on published solvent selection guides because of their low toxicity and preparation from biomass materials [18]. Abraham predictive expressions are reported for *tert*-butyl acetate based on our measured solubility data for acenaphthene, acetylsalicylic acid, anthracene, benzil, benzoic acid, benzoin, 4-*tert*-butylbenzoic acid, 1-chloroanthraquinone, 3-chlorobenzoic acid, 4-chlorobenzoic acid, 2-chloro-5-nitrobenzoic acid, 4-chloro-3-nitrobenzoic acid, 3,4-dichlorobenzoic acid, 3,4-dimethoxybenzoic acid, 3,5-dinitrobenzoic acid, diphenyl sulfone, 2-ethylqnthraquinone, hippuric acid, 2-hydroxybenzoic acid, 2-methoxybenzoic acid, 4-methoxybenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 2-methyl-3-nitrobenzoic acid, 3-methyl-4-nitrobenzoic acid, 4-methyl-3-nitrobenzoic acid, 3-nitrobenzoic acid, 4-nitrobenzoic acid, salicylamide, 3,4,5-trimethoxybenzoic acid, and xanthene. In total, mole fraction solubilities

have been determined for 31 crystalline organic compounds dissolved in *tert*-butyl acetate at 298.15 K.

As part of the current study, we are also revising our existing Abraham model mathematical correlations for both ethyl acetate (dry, anhydrous) [19]:

$$\log P \text{ and } \log (C_{S,organic}/C_{S,water}) = 0.328(0.034) + 0.369(0.057)\mathbf{E} - 0.446(0.080)\mathbf{S} - 0.700(0.069)\mathbf{A} - 4.904(0.113)\mathbf{B} + 4.150(0.033)\mathbf{V} \quad (3)$$
$$(N = 106, SD = 0.165, R^2 = 0.996, F = 4475.1)$$

$$\log K \text{ and } \log (C_{S,organic}/C_{S,gas}) = 0.182(0.026) - 0.352(0.048)\mathbf{E} + 1.316(0.050)\mathbf{S} + 2.891(0.061)\mathbf{A} + 0.916(0.008)\mathbf{L} \quad (4)$$
$$(N = 106, SD = 0.148, R^2 = 0.998, F = 15{,}635.1)$$

and butyl acetate (dry, anhydrous) [19]:

$$\log P \text{ and } \log (C_{S,organic}/C_{S,water}) = 0.248(0.047) + 0.356(0.065)\mathbf{E} - 0.501(0.082)\mathbf{S} - 0.867(0.096)\mathbf{A} - 4.973(0.100)\mathbf{B} + 4.281(0.027)\mathbf{V} \quad (5)$$
$$(N = 73, SD = 0.160, R^2 = 0.998, F = 7380)$$

$$\log K \text{ and } \log (C_{S,organic}/C_{S,gas}) = 0.147(0.040) - 0.414(0.064)\mathrm{E} + 1.212(0.077)\mathbf{S} + 2.623(0.086)\mathbf{A} + 0.954(0.007)\mathbf{L} \quad (6)$$
$$(N = 73, SD = 0.157, R^2 = 0.998, F = 6174.7)$$

as there has been sufficient new experimental data [19–88] published since 2008, when the earlier correlations first appeared, to merit a redetermination of the equation coefficients. Equations (3)–(6) are based on 106 and 73 experimental molar solubility ratios; indirect water-to-alkyl acetate transfer coefficients, *P*; and gas-to-alkyl acetate partition coefficients, *K*, respectively. The updated correlations reported in the current study are based on much larger, more chemically diverse data sets, which include 170 (ethyl acetate) and 108 (butyl acetate) solutes. It is the chemical diversity, as reflected by the solute descriptor values, that defines the area of predictive chemical space over which a derived Abraham correlation can be used. One should not use a mathematical correlation to make predictions for solutes whose descriptor values fall too far outside of the range of values used in determining the equation coefficients.

The words 'dry, anhydrous' after the solvent name indicate that the organic solvent was not in direct contact with water, as would be the case for practical partitioning processes involving the removal of the solute from water with ethyl acetate or butyl acetate as the extracting organic solvent. Abraham model correlations have been published for "wet" ethyl acetate and "wet" butyl acetate in an earlier paper [19]; however, there has not been sufficient new experimental water-to-ethyl acetate and water-to-butyl acetate partition coefficient data to merit updating these existing "wet" Abraham model correlations.

The statistical information associated with Equations (3)–(6) appears immediately below the equation itself and includes the number of experimental data points used in the regression analysis, *N*; the standard deviation, *SD*; the squared correlation coefficient, R^2; and the Fisher F-statistic, *F*. The numerical values contained within parenthesis that immediately follow each equation coefficient are the standard error in the respective calculated coefficient. As an informational item, the $b \times \mathbf{B}$ term is missing in Equations (4) and (6), because both ethyl acetate and butyl acetate lack an acidic hydrogen, and thus, they cannot act as an H-bond donor. The term does appear in Equations (3) and (5), as here, the *b*-coefficients represent the difference in the H-bond acidity of the alkyl acetate solvent(s) and water. Water does possess an H-bond donor character.

2. Experimental Methodology

The crystalline organic solutes selected for the solubility study include 22 carboxylic acids as well as 9 noncarboxylic acid solutes possessing relatedly large **E** and **S** descriptor values. All chemicals used in the current study were purchased from commercial sources

in the highest purity available. Several of the compounds were further purified by recrystallization from either acetone or anhydrous methanol prior to performing the solubility measurements. All solid compounds were dried for two days at 333 K. Purification details and chemical suppliers are given in Table 1, along with the final purities as determined by either a gas–liquid chromatographic analysis (noncarboxylic acid solutes, flame ionization detector) or the non-aqueous acid–base titrimetric method based on a modified procedure recommended by Fritz and Lisicki [89]. Our modified titration procedure replaced benzene with toluene as a component in the titration solvent for health reasons.

Table 1. Chemical sources and final mass fraction purities of chemicals used in the solubility studies.

Chemical	Supplier	Purification Method	Purity (Mass Fraction)
tert-Butyl acetate	TCI America, Portland, OR, USA	Stored over activated molecular sieves and distilled	0.997
1-Chloroanthraquinone	Aldrich Chemical Company, Milwaukee, WI, USA	Recrystallized from anhydrous methanol	0.997
2-Ethylanthraquinone	Aldrich Chemical Company	Recrystallized from anhydrous methanol	0.996
Acenaphthene	Aldrich Chemical Company	Recrystallized from anhydrous methanol	0.997
Benzil	Aldrich Chemical Company	Recrystallized from anhydrous methanol	0.997
Anthracene	Aldrich Chemical Company	Recrystallized from anhydrous acetone	0.997
Acetylsalicylic acid	Aldrich Chemical Company	Dried for two days at 333 K	0.998
Diphenyl sulfone	Aldrich Chemical Company	Recrystallized from anhydrous methanol	0.996
Salicylamide	Aldrich Chemical Company	Recrystallized from anhydrous methanol	0.997
Benzoin	Aldrich Chemical Company	Recrystallized from anhydrous methanol	0.997
Xanthene	Aldrich Chemical Company	Recrystallized from anhydrous methanol	0.996
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
3-Chlorobenzoic acid	Aldrich Chemical Company	Dried for two days at 333 K	0.997
4-Chlorobenzoic acid	Acros Organics, Morris Plains, NJ, USA	Dried for two days at 333 K	0.996
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
Hippuric acid	TCI America	Dried for two days at 333 K	0.997
2-Hydroxybenzoic acid	Aldrich Chemical Company	Dried for two days at 333 K	0.997
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	Acros 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
2-Methyl-3-nitrobenzoic acid	Aldrich Chemical Company	Dried for two days at 333 K	0.997
3-Methyl-4-nitrobenzoic acid	Aldrich Chemical Company	Dried for two days at 333 K	0.997
4-Methyl-3-nitrobenzoic acid	Aldrich Chemical Company	Dried for two days at 333 K	0.998
3-Nitrobenzoic acid	Aldrich Chemical Company	Dried for two days at 333 K	0.996
4-Nitrobenzoic acid	Acros Organics	Dried for two days at 333 K	0.998
3,5-Dinitrobenzoic acid	Aldrich Chemical Company	Dried for two days at 333 K	0.997
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 organic compounds, except for 2-hydroxybenzoic acid and 2-methyl-3-nitrobenzoic acid, were determined using a well-established spectrophotometric method of chemical analysis. Solubilities of 2-hydroxybenzoic acid and 2-methyl-3-nitrobenzoic acid were measured by volumetric acid–base titrations to the phenolphthalein endpoint using a standardized aqueous-sodium hydroxide titrant. In both analytical methods, weighed

aliquots of the saturated solutions were transferred into volumetric (for spectrophotometric method) or Erlenmeyer (for titrimetric method) flasks after an initial three-day equilibration in constant-temperature water at 298.15 ± 0.05 K. The samples were periodically shaken to facilitate mixing and dissolution of the solid solute. In the case of the spectrophotometric determinations, the transferred aliquot was quantitatively diluted with 2-propanol. Additional dilutions were performed if necessary in order for the samples' absorbencies to fall on the Beer–Lambert Law calibration curve, established by graphing the measured absorbances versus the molar concentrations of the nine standard solutions having a known molar solute concentration. All absorbance measurements were recorded on a Milton Roy Spectronic 1000 Plus spectrophotometer. The analysis wavelengths and molar concentration ranges of the standard solutions are reported in Table 2 for each of the analytes, whose solubility was determined by the spectrophotometric method. Attainment of equilibrium was established by performing replicate measurements on the equilibrated samples after two (and in some cases three) additional days of equilibrium. In all instances, the replicate measurements confirmed that equilibrium had been obtained after the initial three-day equilibrium period.

Table 2. Analysis wavelengths and concentration ranges of standard solutions used in the spectrophotometric determination of solubility.

Chemical	Analysis Wavelength	Molar Concentration Range
1-Chloroanthraquinone	337 (nm)	8.79×10^{-5} to 2.93×10^{-4}
2-Ethylanthraquinone	325 (nm)	1.21×10^{-4} to 4.04×10^{-4}
Acenaphthene	289 (nm)	8.05×10^{-5} to 2.68×10^{-4}
Benzil	390 (nm)	5.49×10^{-3} to 1.83×10^{-2}
Anthracene	356 (nm)	6.76×10^{-5} to 2.25×10^{-4}
Acetylsalicylic acid	272 (nm)	4.19×10^{-4} to 1.40×10^{-3}
Diphenyl sulfone	267 (nm)	2.71×10^{-4} to 9.03×10^{-4}
Salicylamide	300 (nm)	1.06×10^{-4} to 3.55×10^{-4}
Benzoin	313 (nm)	1.11×10^{-3} to 3.71×10^{-3}
Xanthene	280 (nm)	1.79×10^{-4} to 5.95×10^{-4}
Benzoic acid	275 (nm)	4.88×10^{-4} to 1.63×10^{-3}
4-*tert*-Butylbenzoic acid	275 (nm)	2.86×10^{-4} to 9.54×10^{-4}
3-Chlorobenzoic acid	280 (nm)	4.99×10^{-4} to 1.66×10^{-3}
4-Chlorobenzoic acid	272 (nm)	4.60×10^{-4} to 1.53×10^{-3}
2-Chloro-5-nitrobenzoic acid	280 (nm)	8.79×10^{-5} to 2.93×10^{-4}
4-Chloro-3-nitrobenzoic acid	292 (nm)	3.72×10^{-4} to 1.34×10^{-3}
3,4-Dichlorobenzoic acid	280 (nm)	4.60×10^{-4} to 1.53×10^{-3}
Hippuric acid	269 (nm)	6.74×10^{-4} to 2.25×10^{-3}
2-Methoxybenzoic acid	295 (nm)	1.61×10^{-4} to 5.37×10^{-4}
4-Methoxybenzoic acid	273 (nm)	9.72×10^{-5} to 3.24×10^{-4}
3,4-Dimethoxybenzoic acid	286 (nm)	9.23×10^{-5} to 3.08×10^{-4}
3,4,5-Trimethoxybenzoic acid	289 (nm)	1.35×10^{-4} to 4.49×10^{-4}
2-Methylbenzoic acid	279 (nm)	4.49×10^{-4} to 1.50×10^{-3}
3-Methylbenzoic acid	280 (nm)	3.97×10^{-4} to 1.32×10^{-3}
3-Methyl-4-nitrobenzoic acid	295 (nm)	1.73×10^{-4} to 5.78×10^{-4}
4-Methyl-3-nitrobenzoic acid	295 (nm)	3.29×10^{-4} to 1.10×10^{-3}
3-Nitrobenzoic acid	280 (nm)	1.51×10^{-4} to 5.06×10^{-4}
4-Nitrobenzoic acid	272 (nm)	4.51×10^{-5} to 1.50×10^{-4}
3,5-Dinitrobenzoic acid	267 (nm)	6.35×10^{-5} to 2.12×10^{-4}

To check for possible solid–solvate formation and/or possible solid-to-solid phase transition during the solution equilibration time, we did determine the melting point temperature of the solid material recovered from each saturated solution after the solubility measurements were performed. As shown in Table 3, the measured point temperature was within experimental error of the melting point temperature of the purchased commercial sample or the recrystallized compound prior to being placed in contact with the *tert*-butyl acetate mono-solvent. No indication of solid–solvate formation or polymorphism was observed.

Table 3. Comparison of the melting point temperatures of the crystalline solutes prior to contact with *tert*-butyl acetate, $T_{mp,initial}$, and of the recovered crystalline solute in equilibrium with the saturated solution, $T_{mp,equilibrated}$.

Solute	$T_{mp,initial}$/K	$T_{mp,equilibrated}$/K
Benzil	368.5 ± 0.5	368.2 ± 0.4
Anthracene	490.3 ± 0.4	490.0 ± 0.5
Acenaphthene	367.0 ± 0.4	367.2 ± 0.5
Xanthene	374.6 ± 0.5	374.3 ± 0.5
1-Chloroanthraquinone	435.4 ± 0.5	435.2 ± 0.4
Benzoic acid	395.6 ± 0.4	395.8 ± 0.4
4-*tert*-Butylbenzoic acid	441.7 ± 0.6	441.6 ± 0.4
3-Chlorobenzoic acid	427.9 ± 0.4	428.1 ± 0.3
4-Chlorobenzoic acid	512.5 ± 0.3	512.8 ± 0.4
3,4-Dichlorobenzoic acid	479.2 ± 0.5	479.1 ± 0.4
3,4-Dimethoxybenzoic acid	454.3 ± 0.4	454.5 ± 0.5
3,4,5-Trimethoxybenzoic acid	445.6 ± 0.6	445.8 ± 0.5
2-Hydroxybenzoic acid	432.7 ± 0.5	432.9 ± 0.5
2-Methoxybenzoic acid	374.7 ± 0.5	374.8 ± 0.4
4-Methoxybenzoic acid	456.6 ± 0.5	456.3 ± 0.4
2-Methylbenzoic acid	376.5 ± 0.4	376.7 ± 0.4
3-Methylbenzoic acid	382.4 ± 0.4	382.5 ± 0.4
2-Methyl-3-nitrobenzoic acid	455.5 ± 0.4	455.2 ± 0.5
3-Methyl-4-nitrobenzoic acid	490.7 ± 0.5	491.0 ± 0.5
4-Methyl-3-nitrobenzoic acid	461.2 ± 0.6	461.6 ± 0.6
3-Nitrobenzoic acid	414.7 ± 0.4	414.4 ± 0.5
4-Nitrobenzoic acid	512.6 ± 0.5	512.5 ± 0.4
3,5-Dinitrobenzoic acid	481.4 ± 0.5	481.3 ± 0.4
2-Chloro-5-nitrobenzoic acid	440.1 ± 0.5	440.4 ± 0.5
4-Chloro-3-nitrobenzoic acid	456.3 ± 0.5	456.5 ± 0.5
2-Ethylanthraquinone	383.9 ± 0.5	384.2 ± 0.5
Diphenyl sulfone	398.2 ± 0.4	397.9 ± 0.5
Acetylsalicylic acid	413.7 ± 0.5	413.3 ± 0.6
Salicylamide	413.2 ± 0.5	413.4 ± 0.4
Benzoin	410.4 ± 0.4	410.7 ± 0.5
Hippuric acid	463.2 ± 0.5	462.8 ± 0.5

3. Results and Discussion

The experimental mole fraction solubilities, $X_{S,organic}$, of the 31 different crystalline organic solutes dissolved in *tert*-butyl acetate are tabulated in the second and fourth columns of Table 4. The numerical values represent the average of 4–7 independent experimental determinations, which were reproducible to within ±2.5% (relative error). We were not able to find, in the published chemical and engineering literature, solubility data for these organic solutes in *tert*-butyl acetate that we could compare our experimental values against. The only published experimental solubility data that we found was for lovastatin. Nti-Gyabaah and coworkers previously had measured the solubility of lovastatin [23] and simvastatin [88] in seven alkyl acetates between 285 K and 313 K using a high-performance liquid chromatographic method of chemical analysis. The solubility data for both lipid-lowering drug molecules will be used in our determination of the Abraham model equation coefficients for *tert*-butyl acetate. Both lovastatin (**S** = 2.730, **B** = 1.760, **V** = 3.2853, and **L** = 15.459) and simvastatin (**S** = 2.550, **B** = 1.860, **V** = 3.4628, and **L** = 15.551) possess large numerical values for several solute descriptors.

Development of a meaningful Abraham model correlation generally requires somewhere between 30 to 40 experimental values [90,91] that cover a sufficient range of solute descriptor values to enable one to make predictions for a large number of additional solutes. In the case of *tert*-butyl acetate, we have the 31 experimental mole fraction solubilities tabulated in Table 3, as well as the mole fraction solubility data for lovastatin [23] and simvastatin [88], which were retrieved from our search of the published literature. There were two additional experimental values that could be used in our regression analysis, and those were the gas-to-*tert*-butyl acetate partition coefficient and water-to-*tert*-butyl acetate transfer coefficient derived from the vapor pressure of *tert*-butyl acetate and the Raoult's law infinite dilution activity coefficient of *tert*-butyl acetate dissolved in itself. By definition, the Raoult's Law infinite dilution activity coefficient of a compound dissolved in itself is unity. The calculation of log *K* and log *P* from activity coefficients is described in greater detail in the published paper [19] that reported the existing Abraham model correlations for ethyl acetate and butyl acetate. In total, we have experimental solubilities and partition coefficients/transfer coefficients for 34 different solutes.

The Abraham model correlates the logarithms of molar solubility ratios, log ($C_{S,organic}/C_{S,water}$) and log ($C_{S,organic}/C_{S,gas}$), and not the mole fraction solubilities, as with our measured data given in Table 4. The tabulated mole fraction solubility data in Table 4 is converted into molar solubilities by dividing $X_{S,organic}$ by the ideal molar volume of the saturated solution (i.e., $C_{S,organic} \approx X_{S,organic}/[X_{S,organic}\ V_{Solute} + (1 - X_{S,organic})\ V_{Solvent}]$). A numerical value of $V_{solvent}$ = 0.13550 L mol^{-1} was used for the molar volume of *tert*-butyl acetate. The numerical values of the molar volumes of the hypothetical subcooled liquid solutes were given in our earlier publications [24,40–42,53–57,92–107], along with the aqueous molar solubilities, $C_{S,water}$, and solute molar gas concentrations, $C_{S,gas}$, needed in obtaining the two molar solubility ratios. Published mole fraction solubilities of lovastatin and simvastatin were converted to molar solubility ratios in a similar fashion. The experimental log ($C_{S,organic}/C_{S,gas}$) and log ($C_{S,organic}/C_{S,water}$) values at 298.15 K for 33 solutes dissolved in *tert*-butyl acetate are listed in Table 5. Also included in Table 5 is the logarithm of the water-to-*tert*-butyl acetate transfer coefficient, log *P*, and gas-to-*tert*-butyl acetate partition coefficient, log *K*, for the solute *tert*-butyl acetate itself.

Once both sets of molar solubility ratios were calculated, we constructed a series of Abraham model log ($C_{S,organic}/C_{S,water}$) and log ($C_{S,organic}/C_{S,gas}$) equations by substituting the numerical solubility ratios and solute descriptors into Equations (1) and (2). Solute descriptors needed in constructing the Abraham model equations are given in Table 6. As an informational note, several of the compounds listed in Table 6 used the alternant hydrogen-bond basicity descriptor, **B°**, in "wet" water-organic solvents when the wet organic solvent contained appreciable quantities of water. For most solutes, **B** and **B°** were numerically equal but did differ mainly for alkylanilines, alkylpyridines, and sulfoxides.

Table 4. Mole fraction solubilities, $X_{S,organic}$, of select crystalline nonelectrolyte organic compounds dissolved in *tert*-butyl acetate at a temperature of 298.15 K and ambient atmospheric pressure of 101 kPa [a].

Chemical Name	$X_{S,organic}$	Chemical Name	$X_{S,organic}$
1-Chloroanthraquinone	0.003494	3,4-Dichlorobenzoic acid	0.01216
2-Ethylanthraquinone	0.02086	2-Hydroxybenzoic acid	0.1187
Acenaphthene	0.09654	Hippuric acid	0.0005241
Benzil	0.09184	2-Methoxybenzoic acid	0.02938
Anthracene	0.003755	4-Methoxybenzoic acid	0.006635
Acetylsalicylic acid	0.02041	3,4-Dimethoxybenzoic acid	0.003625
Diphenyl sulfone	0.02108	3,4,5-Trimethoxybenzoic acid	0.007172
Salicylamide	0.04114	2-Methylbenzoic acid	0.1170
Benzoin	0.006353	3-Methylbenzoic acid	0.1114
Xanthene	0.08530	2-Methyl-3-nitrobenzoic acid	0.02141
Benzoic acid	0.1295	3-Methyl-4-nitrobenzoic acid	0.008034
4-*tert*-Butylbenzoic acid	0.06369	4-Methyl-3-nitrobenzoic acid	0.01549
3-Chlorobenzoic acid	0.04934	3-Nitrobenzoic acid	0.07749
4-Chlorobenzoic acid	0.007404	4-Nitrobenzoic acid	0.006436
2-Chloro-5-nitrobenzoic acid	0.03879	3,5-Dinitrobenzoic acid	0.02331
4-Chloro-3-nitrobenzoic acid	0.01991		

[a] Standard uncertainties and relative uncertainties are $u(T)$ = 0.05 K; $u(p)$ = 5 kPa; and $u_r(x)$ = 0.025.

Table 5. Experimental logarithms of molar solubility ratios; water-to-*tert*-butyl acetate transfer coefficients, log *P*; and gas-to-*tert*-butyl acetate partition coefficients, log *K*, at 298.15 K.

Solute	Log *K* [a]	Log *P* [b]
tert-Butyl acetate	3.53 [c]	2.09
Benzil	8.74	3.87
Anthracene	7.90	4.87
Acenaphthene	6.75	4.39
Xanthene	7.51	5.01
1-Chloroanthraquinone	9.99	3.95
Benzoic acid	6.68	1.54
4-*tert*-Butylbenzoic acid	8.79	3.56
3-Chlorobenzoic acid	7.36	2.22
4-Chlorobenzoic acid	7.10	2.30
3,4-Dichlorobenzoic acid	7.67	2.93
3,4-Dimethoxybenzoic acid	9.37	0.92
3,4,5-Trimethoxybenzoic acid	10.53	1.27
2-Hydroxybenzoic acid	7.23	1.87
2-Methoxybenzoic acid	7.69	0.89
4-Methoxybenzoic acid	8.19	1.49
2-Methylbenzoic acid	6.30	2.00
3-Methylbenzoic acid	7.04	2.06

Table 5. *Cont.*

Solute	Log K [a]	Log P [b]
2-Methyl-3-nitrobenzoic acid	8.65	1.91
3-Methyl-4-nitrobenzoic acid	8.37	2.00
4-Methyl-3-nitrobenzoic acid	9.03	1.72
3-Nitrobenzoic acid	8.37	1.44
4-Nitrobenzoic acid	8.56	1.66
3,5-Dinitrobenzoic acid	9.95	1.65
2-Chloro-5-nitrobenzoic acid	9.00	2.05
4-Chloro-3-nitrobenzoic acid	9.38	2.17
2-Ethylanthraquinone	9.53	4.71
Diphenyl sulfone	10.22	2.83
Acetylsalicylic acid	9.36	0.86
Salicylamide	8.92	1.24
Benzoin	11.07	2.34
Hippuric acid	11.72	−0.55
Lovastatin	18.10	4.09
Simvastatin	18.17	4.23

[a] For the crystalline solutes, the experimental value was log ($C_{S,organic}/C_{S,gas}$). The estimated uncertainty in log ($C_{S,organic}/C_{S,water}$) was 0.02, based on uncertainties in the mole fraction solubilities. [b] For the crystalline solutes the experimental value was log ($C_{S,organic}/C_{S,water}$). The estimated uncertainty in log ($C_{S,organic}/C_{S,water}$) was 0.02, based on uncertainties in the mole fraction solubilities. [c] Log K was calculated based on an activity coefficient of unity for *tert*-butyl acetate dissolved in *tert*-butyl acetate.

Table 6. Solute descriptors of the compounds used in the regression analysis for determining the Abraham model correlations for *tert*-butyl acetate, ethyl acetate, and butyl acetate.

Solute	E	S	A	B	L	V
Radon	0.000	0.000	0.000	0.000	0.877	0.3840
Hydrogen	0.000	0.000	0.000	0.000	−1.200	0.1086
Oxygen	0.000	0.000	0.000	0.000	−0.723	0.1830
Nitrogen	0.000	0.000	0.000	0.000	−0.978	0.2222
Carbon monoxide	0.000	0.000	0.000	0.040	−0.836	0.2220
Sulfur dioxide	0.370	0.660	0.240	0.190	0.778	0.3465
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949
Octane	0.000	0.000	0.000	0.000	3.677	1.2358
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767
Octadecane	0.000	0.000	0.000	0.000	8.722	2.6448
Nonadecane	0.000	0.000	0.000	0.000	9.226	2.7857
Eicosane	0.000	0.000	0.000	0.000	9.731	2.9266

Table 6. *Cont.*

Solute	E	S	A	B	L	V
Docosane	0.000	0.000	0.000	0.000	10.740	3.2084
Tricosane	0.000	0.000	0.000	0.000	11.252	3.3493
Tetracosane	0.000	0.000	0.000	0.000	11.758	3.4902
Octacosane	0.000	0.000	0.000	0.000	13.780	4.0538
2-Methylpentane	0.000	0.000	0.000	0.000	2.503	0.9540
2,4-Dimethylpentane	0.000	0.000	0.000	0.000	2.809	1.0949
2,5-Dimethyhexane	0.000	0.000	0.000	0.000	3.308	1.2358
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.481	1.2358
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454
Ethylcyclhexane	0.263	0.100	0.000	0.000	3.877	1.1272
Propene	0.103	0.080	0.000	0.070	0.946	0.4883
trans-But-2-ene	0.126	0.080	0.000	0.050	1.664	0.6292
Pent-1-ene	0.093	0.080	0.000	0.070	2.047	0.7701
2-Methylprop-1-ene	0.120	0.080	0.000	0.080	1.579	0.6292
3-Methylbut-1-ene	0.063	0.060	0.000	0.050	1.933	0.7701
Hept-1-ene	0.092	0.080	0.000	0.070	3.063	1.0519
Buta-1,2-diene	0.320	0.230	0.000	0.100	1.543	0.5862
2-Methylbuta-1,3-diene	0.313	0.230	0.000	0.100	2.101	0.7271
Hepta-1,6-diene	0.189	0.200	0.000	0.100	3.028	1.0089
Dichloromethane	0.387	0.570	0.100	0.050	2.019	0.4943
Trichloromethane	0.425	0.490	0.150	0.020	2.480	0.6167
Tetrachloromethane	0.458	0.380	0.000	0.000	2.823	0.7391
1,2-Dichloroethane	0.416	0.640	0.100	0.110	2.573	0.6352
1-Chloropropane	0.216	0.400	0.000	0.100	2.202	0.6537
1-Chlorobutane	0.210	0.400	0.000	0.100	2.722	0.7946
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946
Bromoethane	0.366	0.400	0.000	0.120	2.120	0.5654
2-Bromo-2-methylpropane	0.305	0.290	0.000	0.070	2.609	0.8472
Iodomethane	0.676	0.430	0.000	0.120	2.106	0.5077
Iodoethane	0.640	0.400	0.000	0.140	2.573	0.6486
1,1,2-Triflurotrichlroethane	0.010	0.130	0.000	0.000	2.210	0.8107
1,2-Difluorotetrachlroethane	0.227	0.330	0.000	0.020	3.034	0.9154
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810
2-Methylpropionaldehyde	0.144	0.620	0.000	0.450	2.120	0.6879
Propanone	0.179	0.700	0.040	0.490	1.696	0.5470
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284

Table 6. *Cont.*

Solute	E	S	A	B	L	V
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.5450
Diethylamine	0.154	0.300	0.080	0.690	2.395	0.7220
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237
N,*N*-Dimethylformaide	0.367	1.310	0.000	0.740	3.173	0.6468
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.5900
1-Pentanol	0.219	0.420	0.370	0.480	3.106	0.8718
1-Hexanol	0.210	0.420	0.370	0.480	3.610	1.0127
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900
2-Butanol	0.217	0.360	0.330	0.560	2.338	0.7309
2-Methyl-1-propanol	0.217	0.390	0.370	0.480	2.413	0.7309
3-Methyl-1-butanol	0.192	0.390	0.370	0.480	3.011	0.8718
Cyclohexanol	0.460	0.540	0.320	0.570	3.758	0.9040
1,3-Dichloro-2-propanol	0.546	0.930	0.420	0.540	3.650	0.8348
Dimethyl sulfoxide	0.522	1.720	0.000	0.970	3.401	0.6126
Carbon disulfide	0.876	0.260	0.000	0.030	2.370	0.4905
Tetramethyltin	0.324	0.110	0.000	0.100	2.651	1.0431
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573
o-Xylene	0.663	0.560	0.000	0.160	3.939	0.9982
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.9982
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.9982
trans-Stilbene	1.350	1.210	0.000	0.230	7.456	1.5630
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544
Phenanthrene	2.055	1.290	0.000	0.290	7.632	1.4544
Fluoranthene	2.377	1.550	0.000	0.240	8.827	1.5846
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162
Benzoic acid	0.730	0.900	0.590	0.400	4.657	0.9317
2-Hydroxybenzoic acid	0.900	0.850	0.730	0.370	4.732	0.9904
4-Hydroxybenzoic acid	0.930	0.900	0.810	0.560	4.867	0.9904
Methyl 4-hydroxybenzoate	0.900	1.370	0.690	0.450	5.665	1.1313
2-Methylpyridine	0.598	0.750	0.000	0.580	3.422	0.8162
2-Furaldehyde	0.690	1.130	0.000	0.450	3.318	0.6929
Phenylacetic acid	0.730	1.080	0.660	0.570	4.962	1.0726

Table 6. *Cont.*

Solute	E	S	A	B	L	V
4-Hydroxyphenylacetic acid	1.030	1.450	0.940	0.740	5.902	1.1313
4-Ethoxyacetanilide	0.940	1.480	0.480	0.860	6.893	1.4542
Betulin	1.790	2.120	0.700	1.140	17.470	3.8670
3-Nitrophthalic acid	1.360	2.010	1.200	0.890	7.780	1.3212
Acetylsalicylic acid	0.781	1.690	0.710	0.670	6.279	1.2879
3-Chlorobenzoic acid	0.840	0.950	0.630	0.320	5.197	1.0541
4-Chlorobenzoic acid	0.840	1.020	0.630	0.270	4.947	1.0541
3-Nitrobenzoic acid	0.990	1.180	0.730	0.520	5.601	1.1059
4-Nitrobenzoic acid	0.990	1.520	0.680	0.400	5.770	1.1059
3,5-Dinitrobenzoic acid	1.250	1.630	0.700	0.590	6.984	1.2801
4-Chloro-3-nitrobenzoic acid	1.250	1.470	0.700	0.440	6.685	1.2283
2-Chloro-5-nitrobenzoic acid	1.250	1.400	0.670	0.460	6.513	1.2283
2-Methoxybenzoic acid	0.899	1.410	0.450	0.620	5.636	1.1313
4-Methoxybenzoic acid	0.899	1.250	0.620	0.520	5.741	1.1313
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	4.677	1.0726
3-Methylbenzoic acid	0.730	0.890	0.600	0.400	4.819	1.0726
Ketoprofen	1.650	2.260	0.550	0.890	10.527	1.9779
Naproxen	1.510	2.020	0.600	0.670	9.207	1.7821
Haloperidol	1.900	1.390	0.400	1.760	12.819	2.7980
Paracetamol	1.060	1.630	1.040	0.860	6.430	1.1724
4-Nitrobenzyl chloride	1.080	1.350	0.000	0.350	5.806	1.1539
Salicylamide	1.160	1.580	0.610	0.510	5.818	1.0315
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	9.171	1.6512
Monuron	1.140	1.500	0.470	0.780	7.180	1.4768
Diuron	1.280	1.600	0.570	0.700	8.060	1.5992
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209
Diphenyl sulfone	1.570	2.150	0.000	0.700	8.902	1.6051
Hexachlorobenzene	1.490	0.990	0.000	0.000	7.390	1.4508
Hydroquinone	1.063	1.270	1.060	0.570	4.827	0.8338
1,3-Dicyanobenzene	0.890	1.639	0.000	0.561	5.372	1.0258
1,4-Dicyanobenzene	0.870	1.602	0.000	0.470	5.330	1.0258
Benzenesulfonamide	1.130	2.137	0.651	0.647	6.524	1.0971
2-Chlorobenzenesulfonamide	1.220	2.310	0.660	0.623	7.291	1.2195
o-Toluenesulfonamide	1.130	2.157	0.692	0.595	7.076	1.2380
p-Toluenesulfonamide	1.130	2.203	0.680	0.679	7.108	1.2380
Methyl 2-Sulfamoylbenzoate	1.170	2.813	0.664	0.928	8.476	1.4533
2-Chlorothioxanthone	2.226	1.394	0.000	0.556	9.319	1.6581
2-Mercapto-1,3,4-thiadizole	1.166	1.066	0.365	0.457	4.285	0.7224
Dapsone	2.210	3.370	0.800	1.080	11.716	1.8047

Table 6. *Cont.*

Solute	E	S	A	B	L	V
Salicylanilide	1.868	2.161	0.895	0.361	8.915	1.4436
Dimethyl terephthalate	0.788	1.426	0.000	0.567	6.519	1.4288
5,6-Dimethoxy-1-indanone	1.037	1.211	0.000	0.785	6.703	1.4454
Pyrazinamide	1.030	1.458	0.331	0.856	4.976	0.8106
3-Methyl-4-nitrophenol	1.070	1.300	0.740	0.320	5.731	1.0902
2-Ethoxybenzamide	0.910	1.406	0.377	0.952	6.297	1.3133
Chlorpropanamide	1.224	2.234	0.734	0.988	9.712	1.8986
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357
2-Iodoaniline	1.530	1.096	0.130	0.426	5.818	1.0744
4-Iodoaniline	1.530	1.342	0.225	0.400	6.031	1.0744
Nicotinamide	1.010	1.277	0.621	0.958	5.067	0.9317
2-Phenylindole	1.990	1.880	0.420	0.360	9.051	1.5542
Syringic acid	1.070	1.790	0.820	0.900	7.269	1.3896
Kojic acid	1.130	1.589	0.706	0.939	5.594	0.9512
Pyrimethamine	2.230	1.863	0.392	1.101	10.508	1.8458
2-Bromodibenzofuran	2.340	1.778	0.000	0.612	10.781	1.9218
p-Coumaric acid	1.330	1.453	0.841	0.674	6.795	1.2292
2,4-Dinitroaniline	1.430	2.197	0.554	0.310	7.259	1.1646
Terephthaldehyde	1.030	1.235	0.000	0.566	5.235	1.0296
2-Methoxy-4-nitroaniline	1.220	1.680	0.170	0.460	6.474	1.1900
2-Chloro-5-nitroaniline	1.290	1.564	0.268	0.358	6.238	1.1128
1-Methyl-4-(methylsulfonyl)benzene	0.792	1.573	0.000	0.788	6.034	1.2791
1,3-Diphenylguanidine	1.540	1.974	0.585	0.767	9.216	1.7215
Tinidazole	1.400	2.768	0.000	1.348	9.402	1.6959
Sorafenib	2.460	2.913	0.574	1.494	15.998	3.0195
3,4-Dichlorobenzoic acid	0.950	0.920	0.670	0.260	5.623	1.1766
3,4-Dimethoxybenzoic acid	0.950	1.646	0.570	0.755	6.746	1.3309
3,4,5-Trimethoxybenzoic acid	1.001	1.760	0.603	0.850	7.711	1.5309
4-*tert*-Butylbenzoic acid	0.730	1.111	0.551	0.443	6.547	1.4953
Vanillin	0.990	1.336	0.321	0.662	5.703	1.1313
Isovanillin	1.040	1.477	0.308	0.681	5.868	1.1313
2-Ethylanthraquinone	1.410	1.545	0.000	0.557	8.781	1.8106
Benzoin	1.587	2.115	0.196	0.847	9.159	1.6804
Hippuric acid	1.170	1.839	1.207	0.918	7.375	1.3290
2-Methyl-3-nitrobenzoic acid	1.040	1.396	0.541	0.532	6.332	1.2468
3-Methyl-4-nitrobenzoic acid	1.040	1.336	0.525	0.500	6.266	1.2468
4-Methyl-3-nitrobenzoic acid	1.040	1.461	0.659	0.521	6.434	1.2468
Sorbic acid	0.480	0.904	0.528	0.432	4.047	0.9424
Maltol	0.888	1.152	0.212	0.763	4.510	0.8925
o-Acetoacetanisidide	1.190	2.333	0.264	1.025	8.563	1.6108

Table 6. *Cont.*

Solute	E	S	A	B	L	V
Isophthalic acid	1.100	1.210	0.960	0.590	5.988	1.1470
Vanillyl alcohol	1.053	1.817	0.755	0.890	6.464	1.1743
Ethyl vanillin	1.040	1.587	0.411	0.664	6.544	1.2722
Vanillic acid	1.144	1.476	0.826	0.639	6.407	1.1900
3,4-Dichloro-1-nitrobenzene	1.100	1.333	0.000	0.141	5.782	1.1354
2,3-Dichloro-1-nitrobenzene	1.100	1.563	0.000	0.098	6.001	1.1354
3,5-Dinitro-2-methylbenzoic acid	1.310	2.120	0.750	0.650	8.040	1.4210
Xanthone	1.640	1.173	0.000	0.563	7.466	1.4309
Lovastatin	1.230	2.730	0.310	1.760	15.459	3.2853
Simvastatin	1.350	2.550	0.320	1.860	15.551	3.4268
2-Bromo-9-fluorenone	1.840	1.425	0.000	0.399	8.415	1.5472
Benorilate	1.897	2.916	0.484	1.364	12.564	2.2930
Probenecid	1.206	1.951	0.701	1.080	10.369	2.1578
3-Methylflavone-8-carboxylic acid	2.050	1.929	0.485	1.034	10.969	2.0259
Metamitron	1.650	2.248	0.395	1.032	6.777	1.5003

Once the numerical values had been inserted into the equations, the only quantities left without numerical values were the two sets of equation coefficients ($c_{eq\,1}$, $e_{eq\,1}$, $s_{eq\,1}$, $a_{eq\,1}$, $b_{eq\,1}$, $v_{eq\,1}$) and ($c_{eq\,2}$, $e_{eq\,2}$, $s_{eq\,2}$, $a_{eq\,2}$, $b_{eq\,2}$, $l_{eq\,2}$) for the *tert*-butyl acetate mono-solvent. The 34 log ($C_{S,organic}/C_{S,water}$) equations and 34 log ($C_{S,organic}/C_{S,gas}$) equations were solved simultaneously to yield:

$$\begin{gathered}\text{Log}\,(C_{S,organic}/C_{S,water}) = 0.456(0.110) + 0.324(0.090)\,\mathbf{E} - 0.661(0.111)\,\mathbf{S} \\ - 1.068(0.084)\,\mathbf{A} - 4.680(0.228)\,\mathbf{B} + 4.101(0.115)\,\mathbf{V} \\ (\text{with } N = 34,\ SD = 0.100,\ R^2 = 0.994,\ F = 990.6)\end{gathered} \quad (7)$$

$$\begin{gathered}\text{Log}\,(C_{S,organic}/C_{S,gas}) = 0.178(0.088) - 0.444(0.061)\,\mathbf{E} + 1.045(0.090)\,\mathbf{S} \\ + 2.522(0.077)\,\mathbf{A} + 0.964(0.017)\,\mathbf{L} \\ (\text{with } N = 34,\ SD = 0.103,\ R^2 = 0.999,\ F = 5319),\end{gathered} \quad (8)$$

the values of the respective equation coefficients that best describe the logarithms of the observed molar solubility ratios. The $b \times \mathbf{B}$ term is missing in Equation (8), because *tert*-butyl acetate lacks an acidic hydrogen, and thus, it cannot act as an H-bond donor. Both correlations were obtained using the IBM SPSS Statistical 22 commercial software.

The two Abraham model correlations provided a very accurate mathematical description of the observed molar solubility ratios, as evidenced by the near-unity squared correlation coefficients ($R^2 = 0.994$ for Equation (7) and $R^2 = 0.999$ for Equation (8)) and low standard deviations ($SD = 0.100$ log units for Equation (7) and $SD = 0.103$ log units for Equation (8)). Figures 1 and 2 provide a graphical comparison of the experimental data versus back-calculated values based on Equations (8) and (7), respectively. The experimental log ($C_{S,organic}/C_{S,gas}$) values spanned a range of approximately 14.6 log units. A slightly smaller range of approximately 5.6 log units was spanned by the log ($C_{S,organic}/C_{S,water}$) values. As an informational note, Equations (7) and (8) were built using a small dataset containing only 34 compounds. Several of the compounds in the dataset were structurally similar to each other, so there would have been some intercorrelation between their descriptor values. In the case of Equation (8), strong correlations were found between the **B** and **S**, **B** and **L**, and **S** and **L** descriptors. For Equation (7), strong correlations were noted between **B** and **S**,

B and **V**, and **S** and **V**. Intercorrelations would diminish as more experimental values were added to the datasets.

The existing Abraham model correlations for both ethyl acetate and butyl acetate were published in 2008, based on the experimental solubility and infinite dilution activity coefficient data that were available at the time. During the last 10 years, there has been an enormous quantity of experimental solubility data reported for new pharmaceutical compounds, pesticides and herbicides, and important chemical reactants used in industrial manufacturing processes. A recent search of the published chemical literature managed to find experimental mole fraction solubility data for an additional 64 and 35 organic compounds dissolved in ethyl acetate and butyl acetate, respectively. The additional solubility data represent an approximate 50% increase in the number of experimental data points that are now available to update the earlier 2008 correlations. The additional compounds include not only important medicinal compounds (simvastatin, lovastatin, sorafenib, tinidazole, dapsone, chlorpropanamide, benorilate, probenecid), flavoring agents (vanillin, vanillic acid, vanillyl alcohol, ethyl vanillin), and substituted benzoic acid derivatives, but also a wide range of multi-functional organic compounds of varying shapes and sizes. The entire ethyl acetate and butyl acetate datasets are given in Tables 6 and 7, respectively, along with the references from which the data were taken. In order to conserve journal space, the experimental values used in deriving the earlier correlations are referenced to the earlier paper [19] in which Equations (3)–(6) first appeared. Experimental-based solute descriptors of several of the additional compounds are reported for the first time in Table 6. As an additional note, the datasets associated with the Abraham model solvent equations have been used by several research groups [108–114] in developing group contribution approaches, machine learning models, quantitative structure-property relationships, and quantum-mechanical methods for predicting Gibbs energies of solvation and Gibbs energies of transfer for describing the equilibrium partitioning of solutes between two phases. Tables 7 and 8 provide enlarged ethyl acetate and butyl acetate datasets to use in future modelling endeavors.

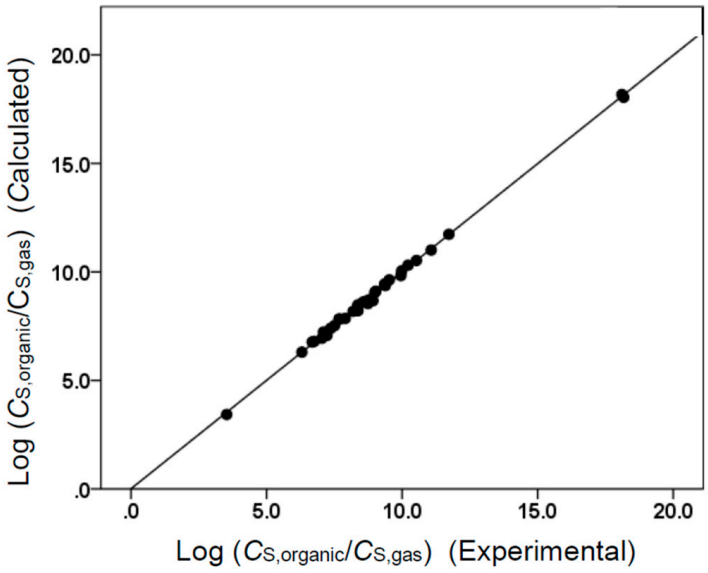

Figure 1. Comparison of observed log ($C_{S,organic}/C_{S,gas}$) data versus back-calculated values based on Equation (8) for *tert*-butyl acetate. The straight line that is drawn corresponds to log ($C_{S,organic}/C_{S,gas}$) (Calculated) = log ($C_{S,organic}/C_{S,gas}$) (Experimental).

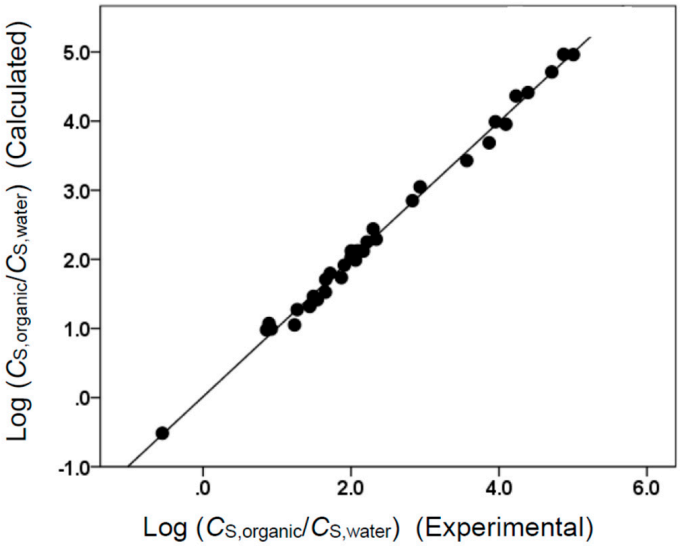

Figure 2. Comparison of observed log ($C_{S,organic}/C_{S,water}$) data versus back-calculated values based on Equation (7) for *tert*-butyl acetate. The straight line that is drawn corresponds to log ($C_{S,organic}/C_{S,water}$) (Calculated) = log ($C_{S,organic}/C_{S,water}$) (Experimental).

Table 7. Experimental logarithms of molar solubility ratios; water-to-ethyl acetate transfer coefficients, log *P*; and gas-to-ethyl acetate partition coefficients, log *K*, at 298.15 K.

Solute	Log *K* [a]	Log *P* [b]	Ref.
Radon	0.810	1.460	[19]
Hydrogen	−1.070	0.650	[19]
Oxygen	−0.660	0.850	[19]
Nitrogen	−0.760	1.040	[19]
Carbon monoxide	−0.600	1.020	[19]
Sulfur dioxide	2.360	0.830	[19]
Ethane	0.490	1.830	[19]
2-Methylpropane	1.580	3.280	[19]
Pentane	2.090	3.790	[19]
Hexane	2.540	4.360	[19]
Heptane	2.980	4.940	[19]
Octane	3.450	5.560	[19]
Nonane	3.910	6.060	[19]
2-Methylpentane	2.410	4.250	[19]
2,4-Dimethylpentane	2.700	4.780	[19]
2,5-Dimethyhexane	3.160	5.180	[19]
2,3,4-Trimethylpentane	3.230	5.110	[19]
Cyclohexane	2.760	3.660	[19]
Ethylcyclhexane	3.540	5.120	[19]
Propene	1.110	2.080	[19]
trans-But-2-ene	2.030	3.140	[19]

Table 7. *Cont.*

Solute	Log K [a]	Log P [b]	Ref.
Pent-1-ene	2.170	3.400	[19]
2-Methylprop-1-ene	1.870	2.730	[19]
3-Methylbut-1-ene	2.010	3.350	[19]
Hept-1-ene	2.980	4.300	[19]
Buta-1,2-diene	2.080	2.530	[19]
2-Methylbuta-1,3-diene	2.410	2.910	[19]
Hepta-1,6-diene	3.370	4.220	[19]
Dichloromethane	2.960	2.000	[19]
Trichloromethane	3.380	2.590	[19]
Tetrachloromethane	3.100	3.290	[19]
1,2-Dichloroethane	3.460	2.190	[19]
1-Chloropropane	2.700	2.460	[19]
1-Chlorobutane	3.160	3.040	[19]
2-Chloro-2-methylpropane	2.610	3.410	[19]
Bromoethane	2.590	2.050	[19]
2-Bromo-2-methylpropane	2.970	3.570	[19]
Iodomethane	2.540	1.890	[19]
Iodoethane	2.960	2.420	[19]
1,1,2-Triflurotrichlroethane	2.490	3.790	[19]
1,2-Difluorotetrachlroethane	3.390	4.030	[19]
Tetrahydrofuran	3.010	0.460	[19]
1,4-Dioxane	3.670	−0.040	[19]
2-Methylpropionaldehyde	2.970	0.870	[19]
Propanone	2.860	0.030	[19]
Butanone	3.260	0.540	[19]
Ethyl acetate	3.300	1.140	[19]
Acetonitrile	3.070	0.220	[19]
Propionitrile	3.430	0.610	[19]
Diethylamine	2.750	−0.240	[19]
Triethylamine	3.130	0.770	[19]
Nitromethane	3.610	0.660	[19]
N,*N*-Dimethylformaide	4.470	−1.260	[19]
Methanol	2.700	−1.040	[19]
Ethanol	3.020	−0.650	[19]
2-Propanol	3.030	−0.450	[19]
Dimethyl sulfoxide	4.880	−2.980	[19]
Carbon disulfide	2.290	2.440	[19]
Tetramethyltin	2.640	4.170	[19]
Benzene	3.240	2.610	[19]
Toluene	3.690	3.040	[19]
trans-Stilbene	8.240	5.720	[85]

Table 7. *Cont.*

Solute	Log K [a]	Log P [b]	Ref.
Acenaphthene	6.920	4.560	[19]
Anthracene	8.150	5.120	[19]
Phenanthrene	8.120	5.320	[19]
Fluoranthene	9.280	5.840	[19]
Pyrene	9.280	5.780	[19]
Chlorobenzene	4.150	3.330	[19]
Aniline	5.490	1.190	[19]
Benzoic acid	6.910	1.790	[19]
2-Hydroxybenzoic acid	7.410	2.020	[19]
4-Hydroxybenzoic acid	8.110	1.330	[19]
Methyl 4-hydroxybenzoate	8.750	1.900	[19]
2-Methylpyridine	4.160	0.760	[19]
2-Furaldehyde	4.620	0.790	[19]
Phenylacetic acid	8.140	1.670	[19]
4-Hydroxyphenylacetic acid	9.950	0.440	[19]
4-Ethoxyacetanilide	9.420	1.420	[19]
Betulin	20.410	10.020	[19]
3-Nitrophthalic acid	12.680	0.010	[19]
Acetylsalicylic acid	9.900	1.330	[19]
3-Chlorobenzoic acid	7.610	2.460	[19]
4-Chlorobenzoic acid	7.410	2.610	[19]
3-Nitrobenzoic acid	8.750	1.820	[19]
4-Nitrobenzoic acid	8.980	2.080	[19]
3,5-Dinitrobenzoic acid	10.410	2.110	[19]
4-Chloro-3-nitrobenzoic acid	9.760	2.550	[19]
2-Chloro-5-nitrobenzoic acid	9.410	2.460	[19]
2-Methoxybenzoic acid	8.180	1.370	[19]
4-Methoxybenzoic acid	8.620	1.920	[19]
2-Methylbenzoic acid	6.530	2.230	[19]
3-Methylbenzoic acid	7.260	2.280	[19]
Ketoprofen	13.760	3.300	[19]
Naproxen	12.500	3.700	[19]
Salicylamide	9.230	1.630	[19]
Benzil	9.040	4.170	[19]
1-Chloroanthraquinone	10.410	4.380	[19]
Monuron	9.580	1.950	[19]
Diuron	10.700	2.700	[19]
Ferrocene	6.020	4.100	[19]
Diphenyl sulfone	10.670	3.280	[19]
Hexachlorobenzene	7.510	6.100	[19]
Docosane	10.010	13.580	[19]

Table 7. *Cont.*

Solute	Log K [a]	Log P [b]	Ref.
Tricosane	10.540	14.260	[19]
Hydroquinone	9.050	0.180	[19]
1,3-Dicyanobenzene	7.209	1.670	[39]
1,4-Dicyanobenzene	7.062	2.055	[34]
Benzenesulfonamide	10.581	0.811	[78]
2-Chlorobenzenesulfonamide	11.478	1.368	[33]
o-Toluenesulfonamide	11.189	1.574	[28]
p-Toluenesulfonamide	11.252	1.163	[74]
Methyl 2-Sulfamoylbenzoate	13.433	0.757	[77]
2-Chlorothioxanthone	9.878	4.789	[35]
2-Mercapto-1,3,4-thiadizole	6.127	0.780	[37]
Dapsone	16.998	1.408	[68]
Salicylanilide	13.001	3.502	[31]
Dimethyl terephthalate	8.015	3.373	[29]
5,6-Dimethoxy-1-indanone	7.722	2.487	[48]
Pyrazinamide	7.348	−0.569	[65]
3-Methyl-4-nitrophenol	8.881	2.550	[81]
2-Ethoxybenzamide	8.405	0.409	[82]
Chlorpropanamide	13.734	2.351	[30]
Thioxanthen-9-one	9.155	4.087	[58]
2-Iodoaniline	6.792	2.623	[46]
4-Iodoaniline	7.513	2.498	[46]
Nicotinamide	7.874	−1.148	[22]
2-Phenylindole	11.533	4.638	[44]
Syringic acid	11.199	0.700	[80]
Kojic acid	8.951	−1.167	[64]
Pyrimethamine	12.767	2.501	[47]
2-Bromodibenzofuran	11.704	5.505	[50]
p-Coumaric acid	10.061	1.187	[21]
2,4-Dinitroaniline	10.930	2.868	[51]
Terephthaldehyde	6.294	1.703	[52]
2-Methoxy-4-nitroaniline	8.569	2.742	[25]
2-Chloro-5-nitroaniline	8.427	2.912	[20]
1-Methyl-4-(methylsulfonyl)benzene	7.731	1.549	[79]
1,3-Diphenylguanidine	12.388	2.986	[45]
Tinidazole	12.262	0.329	[38]
Sorafenib	19.501	4.760	[36]

Table 7. *Cont.*

Solute	Log K [a]	Log P [b]	Ref.
3,4-Dichlorobenzoic acid	7.939	3.199	[40]
3,4-Dimethoxybenzoic acid	9.680	1.410	[41]
3,4,5-Trimethoxybenzoic acid	11.012	1.757	[42]
4-*tert*-Butylbenzoic acid	8.951	3.726	[53]
Vanillin	7.739	1.311	[65]
Isovanillin	7.995	1.157	[86]
2-Ethylanthraquinone	9.925	5.111	[24]
Benzoin	11.512	2.781	[57]
Hippuric acid	12.276	0.001	[49]
2-Methyl-3-nitrobenzoic acid	8.951	2.214	[54]
3-Methyl-4-nitrobenzoic acid	8.743	2.379	[55]
4-Methyl-3-nitrobenzoic acid	9.485	2.173	[56]
Sorbic acid	6.340	1.429	[60]
Maltol	6.129	−0.045	[75]
o-Acetoacetanisidide	11.661	1.427	[63]
Isophthalic acid	9.193	0.933	[69]
Vanillyl alcohol	10.308	−0.114	[73]
Ethyl vanillin	9.075	1.734	[72]
Vanillic acid	9.983	1.317	[70]
3,4-Dichloro-1-nitrobenzene	6.712	4.006	[61]
2,3-Dichloro-1-nitrobenzene	7.280	4.187	[61]
3,5-Dinitro-2-methylbenzoic acid	12.058	2.102	[59]
Xanthone	8.034	3.624	[43]
Lovastatin	18.336	4.424	[23]
Simvastatin	18.400	4.749	[88]
2-Bromo-9-fluorenone	9.139	4.841	[67]
Benorilate	16.329	2.278	[32]
Probenecid	13.750	2.976	[76]
3-Methylflavone-8-carboxylic acid	13.426	3.198	[84]
Metamitron	11.823	0.916	[87]

[a] For the crystalline solutes, the experimental value is log ($C_{S,organic}/C_{S,gas}$). [b] For the crystalline solutes, the experimental value is log ($C_{S,organic}/C_{S,water}$).

Analysis of the experimental values in Tables 6 and 7 in accordance with the Abraham general solvation model yielded the following mathematical correlations:

For Ethyl Acetate:

$$\begin{gathered}\text{Log}\,(C_{S,organic}/C_{S,water}) = 0.328(0.025) + 0.314(0.033)\,\mathbf{E} - 0.348(0.039)\,\mathbf{S} \\ - 0.847(0.043)\,\mathbf{A} - 4.899(0.058)\,\mathbf{B} + 4.142(0.025)\,\mathbf{V} \\ (\text{with } N = 170,\ SD = 0.144,\ R^2 = 0.996,\ F = 7548)\end{gathered} \quad (9)$$

$$\begin{gathered}\text{Log}\,(C_{S,organic}/C_{S,gas}) = 0.171(0.020) - 0.403(0.030)\,\mathbf{E} + 1.428(0.028)\,\mathbf{S} \\ + 2.726(0.038)\,\mathbf{A} + 0.914(0.006)\,\mathbf{L} \\ (\text{with } N = 170,\ SD = 0.131,\ R^2 = 0.999,\ F = 42942)\end{gathered} \quad (10)$$

For Butyl Acetate:

$$\text{Log}\,(C_{S,organic}/C_{S,water}) = 0.289(0.037) + 0.336(0.041)\,\mathbf{E} - 0.501(0.050)\,\mathbf{S} - 0.913(0.054)\,\mathbf{A} - 4.964(0.063)\,\mathbf{B} + 4.262(0.021)\,\mathbf{V} \quad (11)$$
$$(\text{with } N = 108,\ SD = 0.140,\ R^2 = 0.998,\ F = 11519)$$

$$\text{Log}\,(C_{S,organic}/C_{S,gas}) = 0.154(0.034) - 0.439(0.041)\,\mathbf{E} + 1.223(0.041)\,\mathbf{S} + 2.586(0.056)\,\mathbf{A} + 0.953(0.006)\,\mathbf{L} \quad (12)$$
$$(\text{with } N = 108,\ SD = 0.148,\ R^2 = 0.999,\ F = 17169)$$

As, before, the $b \times \mathbf{B}$ term was missing in Equations (10) and (12), neither ethyl acetate nor butyl acetate could act as an H-bond donor. Neither solvent molecule possesses an acidic hydrogen. All four derived correlations provided a reasonably accurate description of the observed solubility and partition coefficient data, as numerically reflected by the near unity squared correlation coefficient and the relatively small standard deviations. The descriptive ability is further illustrated in Figures 3–6. For most of the solute molecules considered, the graphed points fell near the drawn straight line, indicating a near-perfect back-calculation.

Table 8. Experimental logarithms of molar solubility ratios; water-to-butyl acetate transfer coefficients, log *P*; and gas-to-butyl acetate partition coefficients, log *K*, at 298.15 K.

Solute	Log *K* [a]	Log *P* [b]	Ref.
Hydrogen	−1.100	0.620	[19]
Nitrogen	−0.800	1.000	[19]
Nitrous oxide	0.720	0.950	[19]
Carbon monoxide	−0.640	0.980	[19]
Pentane	2.150	3.850	[19]
Hexane	2.630	4.450	[19]
Heptane	3.100	5.060	[19]
Octane	3.560	5.670	[19]
Nonane	4.020	6.170	[19]
2-Methylpentane	2.490	4.330	[19]
2,4-Dimethylpentane	2.790	4.870	[19]
2,5-Dimethylhexane	3.270	5.290	[19]
2,3,4-Trimethylpentane	3.340	5.220	[19]
Cyclohexane	2.870	3.770	[19]
Ethylcyclohexane	3.660	5.240	[19]
1-Heptene	3.140	4.360	[19]
1,6-Heptadiene	3.240	4.090	[19]
Carbon tetrachloride	3.120	3.310	[19]
Butyl acetate	4.090	2.150	[19]
2-Butanol	3.590	0.200	[19]
2-Methyl-1-propanol	3.550	0.250	[19]
1-Propanol	3.410	0.150	[19]
1-Pentanol	4.600	1.250	[19]
3-Methyl-1-butanol	4.240	1.000	[19]

Table 8. *Cont.*

Solute	Log K [a]	Log P [b]	Ref.
1-Hexanol	5.010	1.780	[19]
Cyclohexanol	5.180	1.170	[19]
1,3-Dichloro-2-propanol	5.560	0.380	[19]
Benzene	2.840	2.210	[19]
Toluene	4.030	3.380	[19]
o-Xylene	4.560	3.820	[19]
m-Xylene	4.440	3.830	[19]
p-Xylene	4.470	3.880	[19]
Octadecane	8.750	11.790	[19]
Nonadecane	9.280	12.490	[19]
Eicosane	9.470	12.780	[19]
Docosane	10.360	13.930	[19]
Tricosane	10.930	14.650	[19]
Tetracosane	11.260	15.100	[19]
Octacosane	13.090	17.430	[19]
Anthracene	8.160	5.130	[19]
Pyrene	9.290	5.790	[19]
Fluoranthene	9.270	5.830	[19]
Acenaphthene	6.910	4.550	[19]
Phenanthrene	8.090	5.290	[19]
Methyl 4-hydroxybenzoate	8.680	1.840	[19]
Benzoic acid	6.810	1.710	[19]
2-Hydroxybenzoic acid	7.340	1.950	[19]
4-Hydroxybenzoic acid	7.890	1.110	[19]
trans-Stilbene	8.210	5.690	[85]
Diuron	10.610	2.610	[19]
Monouron	9.390	1.760	[19]
Hexachlorobenzene	7.620	6.120	[19]
Diphenyl sulfone	10.440	3.050	[19]
4-Nitrobenzyl chloride	7.090	3.320	[19]
Paracetamol	10.380	−0.520	[19]
Ferrocene	6.010	4.243	[27]
3-Chlorobenzoic acid	7.500	2.350	[19]
4-Chlorobenzoic acid	7.210	2.410	[19]
3,4-Dichlorobenzoic acid	7.911	3.171	[40]
3-Nitrobenzoic acid	8.530	1.600	[19]
4-Nitrobenzoic acid	8.760	1.860	[19]
3,5-Dinitrobenzoic acid	10.180	1.880	[19]
3,5-Dinitro-2-methylbenzoic acid	11.853	1.897	[59]
2-Methylbenzoic acid	6.420	2.120	[19]

Table 8. *Cont.*

Solute	Log K [a]	Log P [b]	Ref.
3-Methylbenzoic acid	7.100	2.120	[19]
3-Methyl-4-nitrobenoic acid	8.635	2.271	[55]
Naproxen	12.200	3.400	[19]
Acetylsalicylic acid	9.580	1.080	[19]
2-Methoxybenzoic acid	7.880	1.080	[19]
4-Methoxybenzoic acid	8.410	1.710	[19]
3,4-Dimethoxybenzoic acid	9.462	1.192	[41]
3,4,5-Trimethoxybenzoic acid	10.757	1.501	[42]
Benzil	8.930	4.060	[19]
4-Nitroaniline	9.290	2.100	[19]
Haloperidol	14.320	3.020	[19]
Hydroquinone	8.960	0.140	[19]
1-Chloroanthraquinone	10.290	4.260	[19]
Salicylamide	9.010	1.410	[19]
4-Chloro-3-nitrobenzoic acid	9.390	2.360	[20]
2-Chloro-5-nitrobenzoic acid	9.130	2.180	[20]
Lovastatin	18.279	4.267	[23]
2-Ethylanthraquinone	9.865	5.042	[24]
Simvastatin	18.677	4.678	[88]
Thioxanthen-9-one	9.335	4.051	[58]
Benzoin	11.305	2.574	[57]
Maltol	6.033	−0.156	[75]
Nicotinamide	7.727	−1.295	[26]
2-Methyl-3-nitrobenzoic acid	8.847	2.110	[54]
4-*tert*-Butylbenzoic acid	8.825	3.600	[53]
o-Acetoacetanisidide	11.407	1.173	[63]
Xanthone	7.940	3.530	[43]
Vanillyl alcohol	9.948	−0.474	[73]
Hippuric acid	12.082	−0.193	[49]
2-Ethoxybenzamide	8.310	0.314	[83]
Chlorpropanamide	13.479	2.096	[30]
4-Methyl-3-nitrobenzoic acid	9.342	2.063	[56]
Dapsone	16.416	0.826	[68]
Salicylanilide	12.785	3.286	[31]
Dimethyl terephthalate	7.867	3.225	[29]
5,6-Dimethoxy-1-indanone	7.398	2.163	[48]
Pyrazinamide	7.108	−0.809	[65]
3-Methyl-4-nitrophenol	8.746	2.415	[81]
Tinidazole	11.922	−0.011	[38]
2-Bromo-9-fluorenone	9.134	4.836	[67]
Benorilate	15.974	1.925	[32]

Table 8. *Cont.*

Solute	Log K [a]	Log P [b]	Ref.
Probenecid	13.554	2.780	[76]
3-Methylflavone-8-carboxylic acid	13.151	2.923	[84]
Metamitron	11.593	0.686	[87]

[a] For the crystalline solutes, the experimental value is log ($C_{S,organic}/C_{S,gas}$). [b] For the crystalline solutes, the experimental value is log ($C_{S,organic}/C_{S,water}$).

We further note that the numerical values of the equation coefficients changed slightly from the values given in the earlier 2008 correlations (See Equations (3)–(6)). The change is likely reflected by the addition of several large, highly basic molecules (sorafenib, **B** = 1.494, **V** = 3.0195; lovastatin, **B** = 1.760, **V** = 3.2853; simvastatin, **B** = 1.860, **V** = 3.4268) to the datasets. Prior to the inclusion of an additional 64 compounds, betulin (**B** = 1.140) was the only compound in the ethyl acetate dataset having a B-solute descriptor that exceeded unity. It is important to periodically update existing correlations as new experimental data become available in order to expand the predictive area of chemical space. Ethyl acetate and, to a lesser extent, butyl acetate are solvents that researchers use in performing solubility studies on new drug molecules. These are also two organic solvents that we routinely use in calculating solute descriptor values. Datasets used in determining the Abraham model correlations need to contain solutes that possess the molecular size, polarity, and lipophilicity common to the newly approved medicinal compounds, if the correlations are to be used in calculating solute descriptors of these compounds. Newer drug molecules tend to be larger and more lipophilic and possess a greater H-bond acceptor capability than older drugs [115]. The predictive area of chemical space covered by the Abraham model correlations needs to keep pace with the molecular properties of today's modern drug molecules.

Many of the compounds used in chemical manufacturing processes will have solute descriptors that fall within these ranges. Currently solute descriptors are readily available on the UFZ-LSER internet website [116] for more than 8500 different organic compounds. If not available, there are group contribution methods [117,118], as well as machine learning models [108,119], that can be used to estimate the desired descriptor values. The estimation requires simply inputting the canonical SMILES code of the desired solute into the software program found at either the UFZ-LSER website or at the RMG-MIT website link embedded in [89] in the published paper [108].

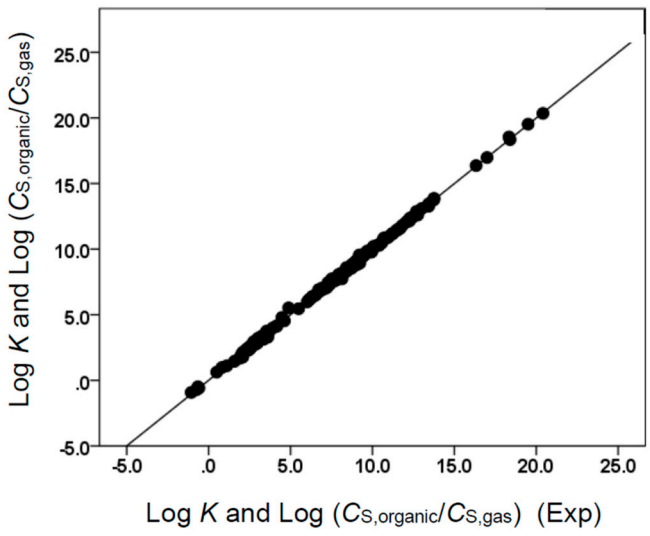

Figure 3. Comparison of observed log K and log ($C_{S,organic}/C_{S,gas}$) data versus back-calculated values based on Equation (10) for ethyl acetate. The straight line that is drawn corresponds to log K and log ($C_{S,organic}/C_{S,gas}$) (Calc) = log K and log ($C_{S,organic}/C_{S,gas}$) (Exp).

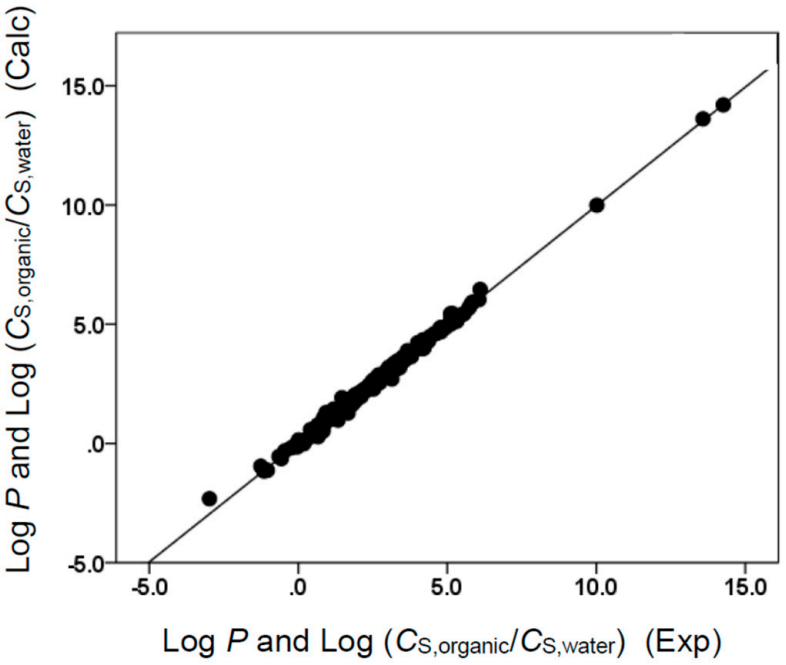

Figure 4. Comparison of observed log P and log ($C_{S,organic}/C_{S,water}$) data versus back-calculated values based on Equation (9) for ethyl acetate. The straight line that is drawn corresponds to log P and log ($C_{S,organic}/C_{S,water}$) (Calc) = log P and log ($C_{S,organic}/C_{S,water}$) (Exp).

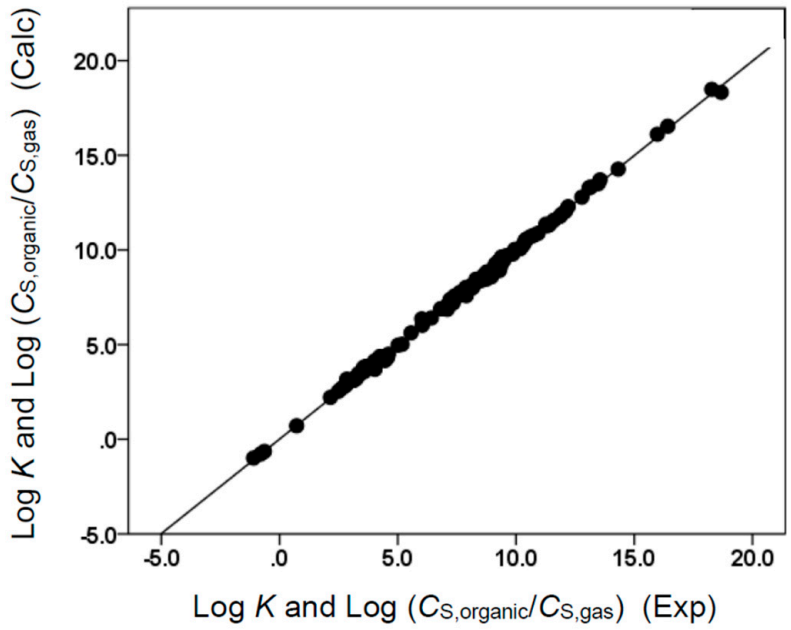

Figure 5. Comparison of observed log K and log ($C_{S,organic}/C_{S,gas}$) data versus back-calculated values based on Equation (12) for butyl acetate. The straight line that is drawn corresponds to log K and log ($C_{S,organic}/C_{S,gas}$) (Calc) = log K and log ($C_{S,organic}/C_{S,gas}$) (Exp).

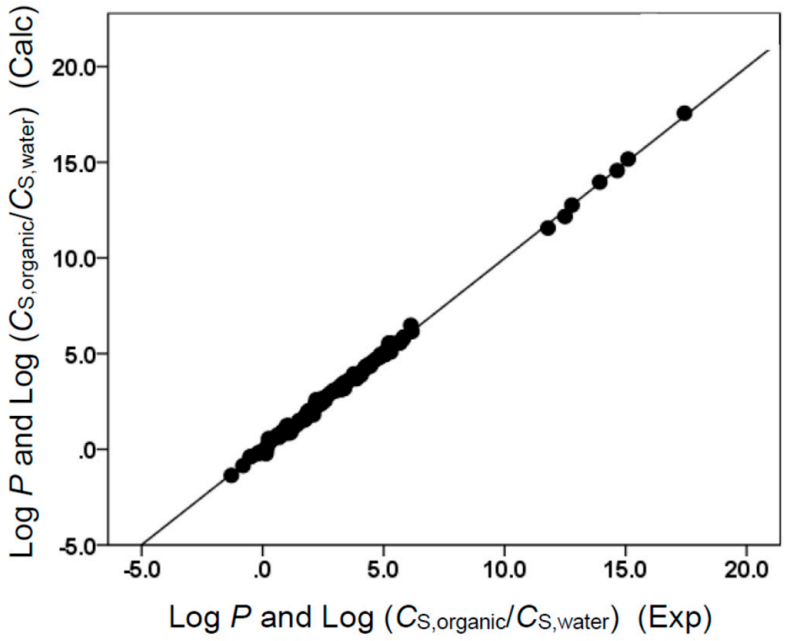

Figure 6. Comparison of observed log P and log ($C_{S,organic}/C_{S,water}$) data versus back-calculated values based on Equation (11) for butyl acetate. The straight line that is drawn corresponds to log P and log ($C_{S,organic}/C_{S,water}$) (Calc) = log P and log ($C_{S,organic}/C_{S,water}$) (Exp).

4. Conclusions

Mathematical expressions based upon the Abraham general solvation parameter model were obtained for predicting the solute transfer of molecular organic compounds and inorganic gases into three alkyl acetate mono-solvents (*tert*-butyl acetate, ethyl acetate, and butyl acetate). The predictive expressions for the three alkyl acetate solvents were determined using chemically diverse datasets, which contained 34, 170, and 108 solutes of various molecular sizes and shapes, polarities, and hydrogen-bonding characteristics. The mathematical correlations presented in the current study describe the observed solubility ratios of solutes dissolved in *tert*-butyl acetate, ethyl acetate, and butyl acetate to within an overall standard deviation of 0.15 log units or less. Based on our past experience using the Abraham model, we fully expect the derived mathematical expressions to provide comparable predictions for the solubility and partitioning behavior of additional organic solutes in the three fore-mentioned solvents, provided, of course, that the descriptor values of the additional solutes fall within the range of values used in deriving the respective predictive expression. Many of the compounds used in chemical manufacturing processes will have solute descriptors that fall within these ranges.

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