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Gas-solvent and water-solvent partition of trans-stilbene at 298 K



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ABSTRACT

We start with literature data on gas to solvent partition of trans-stilbene, as $\log K$, for 52 solvents. The $\log K$ values can be converted into corresponding water to solvent partitions, as $\log P$, through the stilbene gas to water partition coefficient, and lead, with four additional equations, to a set of 108 simultaneous equations that can be solved to yield descriptors for stilbene with a standard deviation of no more than 0.096 \log units. This represents statistically the best analysis of stilbene solubility to date. The stilbene descriptors can be combined with equation coefficients to give predictions of stilbene gas to solvent partition and water to solvent partition for numerous dry solvents, wet (water saturated) solvents and ionic liquid solvents, as well as predictions of environmental and biological processes involving styrene.

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1. Introduction

trans-Stilbene, or just stilbene, is such an important chemical that its physicochemical properties have been widely studied. Stilbenes have unique properties, including fluorescence and phosphorescence and stilbene itself is a precursor to derivatives used as dyes, optical brighteners and scintillators. Amongst the physicochemical properties studied are those dealing with the solubility of stilbene in a range of organic solvents [1–6]. The solubility of gaseous stilbene has been of particular interest, usually in terms of K, the vapour to solvent partition coefficient (sometimes referred to as L). If concentrations of a solute in the gas phase and in solution are described in the same units, say mol dm^{-3} , then K is dimensionless. In Table 1 we summarise results from various equations that correlate the solubility of stilbene in solvents in terms of the standard deviation between observed and calculated values, SD. The methods include Linear Free Energy Relationships, LFER, Linear Solvation Energy Relationships, LSER, Quantitative Structure-Property Relationships, QPSR, and Mobile Order Theory, MOT. Tulp et al. [5] do not give values of SD. Taking into account the number of independent variables, the QSPR method of Katritzky et al. [4] seems to provide the best fit of experimental and calculated values. Our own analysis [2] used only 20 solvents, so that now the total number of solvents has reached over 50, we thought it useful to apply our previous methods [2] to this larger data set. In addition to calculations of log K, our method provides also an equation for the calculation of water-solvent partition coefficients, as log *P*. For practical purposes, the latter is probably more useful than values of log *K*.

2. Methods

We have already shown [7–9] that two general linear free energy relationships, Eqs. (1) and (2), can be used for the transfer of neutral solutes from water to organic solvents and from the gas phase to organic solvents. There have been several reviews of our method [7,8,10–12]. In brief it is as follows. The dependent variable in Eq. (1) is $\log P$, where P is the molar water to solvent partition coefficient for a solute in a series of solvents, and in Eq. (2) is $\log K$ where K is the dimensionless gas phase to solvent partition coefficient for a given solute in a series of solvents.

$$Log P = c + e\mathbf{E} + s\mathbf{S} + a\mathbf{A} + b\mathbf{B} + v\mathbf{V}$$
 (1)

$$Log K = c + e\mathbf{E} + s\mathbf{S} + a\mathbf{A} + b\mathbf{B} + l\mathbf{L}$$
 (2)

In Eqs. (1) and (2) the independent variables, or descriptors, are properties of the neutral solutes as follows [7–12]: **E** is the solute excess molar refraction in cm³ mol⁻¹/10, **S** is the solute dipolarity/polarizability, **A** is the overall solute hydrogen bond acidity, **B** is the overall solute hydrogen bond basicity, **V** is McGowan's characteristic molecular volume in cm³ mol⁻¹/100 and **L** is the logarithm of the gas to hexadecane partition coefficient at 298 K. The coefficients in Eq. (1) and Eq. (2) are shown in Table 2 for partition from water to the relevant solvents that we shall consider [5,6].

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Table 1 Results from equations for the calculation of $\log K$ for partition of *trans*-stilbene from the gas phase to various solvents at 298 K.

Reference	N	SD
Fletcher et al. [1], MOT	20	0.134 ^a
Abraham et al. [2], LFER	17	0.085
Roy et al. [3], MOT	34	0.133 ^a
Katritzky et al. [4], QSPR	52	0.130
Yousefinejad et al. [6], QSPR	44	0.165
Yousefinejad et al. [6], LSER	42	0.206
This work, LFER	52	0.098

^a The SD values are for mol fraction solubilities of the solid.

The independent variables, or descriptors, are properties of the solutes. If these are not known for a particular solute, a set of simultaneous equations can be set up consisting of known values of $\log P$ and $\log K$ for the solute, and the known coefficients of the corresponding equations. These simultaneous equations can then be solved to yield the required solute descriptors. The relationship between $\log P$ and $\log K$ is given as Eq. (3), where Kw is the solute gas to water partition coefficient. Eq. (3) is absolutely vital as it enables experimental values of $\log P$ to be converted into $\log K$, and experimental values of $\log K$ to be converted into $\log P$.

$$K = P^*Kw \text{ or } logK = logP + logKw$$
(3)

Table 2Coefficients in Eqs. (1) and (2) for a number of solvents, and observed and calculated values of log *P* and log *K* for *trans*-stilbene at 298 K.^a

Solvent, Eq. (1) C e S a b I V C C						
Hexane	a b 1	а	S	е	С	Solvent, Eq. (1)
Helpane	-3.560 -4.594 C	-3.560	-1.159	0.523	e 0.199	Tetrachloromethan
Octane 0.231 0.738 -1.840 -3.685 -4.907 0 4.502 4.482 4 Nonane 0.240 0.619 -1.713 -3.532 -4.921 0 4.476 4 Decane 0.186 0.722 -1.741 -3.449 -4.970 0 4.476 4 Hexadecane 0.087 0.667 -1.617 -3.587 -4.899 0 4.433 4 Cyclobctane 0.126 0.782 -1.678 -3.740 -4.929 0 4.528 4 5 Methylcyclohexane 0.246 0.782 -1.982 -3.517 -4.293 0 4.528 4 6 5 0.026 5 5 6 5 0.026 5 5 1.737 -3.677 -4.663 0 4.655 4 4 1 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	-3.578 —4.939 C	-3.578	-1.710	0.560	0.333	Hexane
Nonane		-3.571	− 1.755	0.634	0.297	Heptane
Decane	-3.685 -4.907 C	-3.685	-1.840	0.738	0.231	Octane
Hexadecane	-3.532 -4.921 C	-3.532	-1.713	0.619	0.240	Nonane
Cyclochxane 0.159 0.784 -1.678 -3.740 -4.929 0 4.577 5 Methylcyclohexane 0.246 0.782 -1.982 -3.517 -4.293 0 4.528 4. Cyclootane a -0.123 0.677 -1.697 -3.519 -5.568 0 5.026 5. t-Butylcyclohexane a 0.172 0.759 -2.025 -2.971 -4.663 0 4.655 4. Isooctane a 0.282 0.469 -1.303 -3.661 -5.126 0 4.107 4. Squalane a 0.282 0.469 -1.303 -3.661 -5.126 0 4.107 4. Senzene 0.142 0.464 -0.588 -3.099 -4.625 0 4.491 6. Toluene 0.125 0.431 -0.644 -3.002 -4.748 0 4.532 5. p-Xylene 0.166 0.477 -0.812 -2.9391 -4.961 0 4.532 5. <td>-3.449 —4.970 C</td> <td>-3.449</td> <td>-1.741</td> <td>0.722</td> <td>0.186</td> <td>Decane</td>	-3.449 —4.970 C	-3.449	-1.741	0.722	0.186	Decane
Methylcyclohexane 0.246 0.782 -1.982 -3.517 -4.293 0 4.528 4 Cyclooctane a -0.123 0.677 -1.697 -3.519 -5.568 0 5.026 5. Lebulycyclohexane a 0.172 0.759 -2.025 -2.971 -4.663 0 4.655 4 Isooctane 0.318 0.555 -1.737 -3.677 -4.864 0 4.417 4 Squalane a 0.282 0.469 -1.303 -3.661 -5.126 0 4.107 4 Benzene 0.142 0.464 -0.588 -3.099 -4.625 0 4.491 6 Toluene 0.122 0.377 -0.603 -2.981 -4.961 0 4.524 5 m-Xylene 0.166 0.477 -0.812 -2.939 -4.874 0 4.532 5 Ethylbenze 0.065 0.381 -0.521 -3.183 -4.700 0 4.614 6 <td>-3.587 —4.869 O</td> <td>-3.587</td> <td>-1.617</td> <td>0.667</td> <td>0.087</td> <td>Hexadecane</td>	-3.587 —4.869 O	-3.587	-1.617	0.667	0.087	Hexadecane
Cyclooctane a -0.123 0.677 -1.697 -3.519 -5.568 0 5.026 5 t-Butylcyclohexane a 0.172 0.759 -2.025 -2.971 -4.663 0 4.655 4.4 Isooctane 0.318 0.555 -1.737 -3.677 -4.864 0 4.417 4 Squalane a 0.282 0.469 -1.303 -3.661 -5.126 0 4.107 4 Benzene 0.142 0.464 -0.588 -3.099 -4.625 0 4.491 6 Toluce 0.125 0.431 -0.644 -3.002 -4.748 0 4.534 5 m-Xylene 0.166 0.477 -0.812 -2.939 -4.874 0 4.535 5 Ethylbenzene 0.093 0.467 -0.723 -3.001 -4.844 0 4.514 5 Chlorobenzene 0.093 0.467 -0.723 -3.001 -4.844 0 4.514 5	-3.740 -4.929 C	-3.740	-1.678	0.784	0.159	Cyclohexane
t-Buylcyclohexane a 0.172 0.759	-3.517 -4.293 C	-3.517	-1.982	0.782	0.246	Methylcyclohexane
Sooctane	-3.519 -5.568 C	-3.519	-1.697	0.677	-0.123	Cyclooctane a
Squalane a 0.282 0.469 -1.303 -3.661 -5.126 0 4.107 4.8 Benzene 0.142 0.464 -0.588 -3.099 -4.625 0 4.491 6 Toluene 0.125 0.431 -0.644 -3.002 -4.748 0 4.524 5 m-Xylene 0.122 0.377 -0.603 -2.981 -4.961 0 4.535 5 p-Xylene 0.166 0.477 -0.812 -2.939 -4.874 0 4.532 5 Ethylbenzene 0.093 0.467 -0.723 -3.001 -4.844 0 4.514 5 Chlorobenzene 0.065 0.381 -0.521 -3.183 -4.700 0 4.614 6 Methanol 0.226 0.471 -1.035 0.326 -3.596 0 3.857 4 Ethanol 0.129 0.247 -3.767 0 3.886 4 Butan-1-ol 0.165	-2.971 -4.663 C	-2.971	-2.025	0.759	a 0.172	t-Butylcyclohexane
Benzene	-3.677 —4.864 C	-3.677	-1.737	0.555	0.318	Isooctane
Benzene	-3.661 -5.126 C	-3.661	-1.303	0.469	0.282	Squalane a
m-Xylene 0.122 0.377 -0.603 -2.981 -4.961 0 4.535 5.5 p-Xylene 0.166 0.477 -0.812 -2.939 -4.874 0 4.532 5.5 Ethylbenzene 0.093 0.467 -0.723 -3.001 -4.844 0 4.514 5.5 Chlorobenzene 0.065 0.381 -0.521 -3.183 -4.700 0 4.614 6.6 Methanol 0.276 0.334 -0.714 0.243 -3.320 0 3.549 4.6 Ethanol 0.222 0.471 -1.035 0.326 -3.596 0 3.857 4.6 Propan-1-ol 0.139 0.405 -1.029 0.247 -3.767 0 3.986 4.8 Butan-1-ol 0.165 0.401 -1.011 0.056 -3.958 0 4.044 4 Hexan-1-ol 0.115 0.492 -1.164 0.054 -3.978 0 4.131 4	-3.099 -4.625 C	-3.099	-0.588	0.464	0.142	
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	-0.618 -5.097 0	-0.618	-0.817	0.307	r 0.341	Methyl t-butyl ethe
Diovane 0.008 0.3500.0830.5564.826 0 4.172 5	-0.236 —4.934 0	-0.236	-0.392	0.372	0.207	Tetrahydrofuran
DIOMAIR 0.030 0.030 -0.000 -4.020 0 4.1/2 3.	-0.556 -4.826 0	-0.556	-0.083	0.350	0.098	Dioxane
Methyl acetate 0.351 0.223 -0.150 -1.035 -4.527 0 3.972 5.	-1.035 -4.527 C	-1.035	-0.150	0.223	0.351	Methyl acetate
Ethyl acetate 0.328 0.369 -0.446 -0.700 -4.904 0 4.150 5.	-0.700 -4.904 C	-0.700	-0.446	0.369	0.328	Ethyl acetate
Butyl acetate 0.248 0.356 -0.501 -0.867 -4.973 0 4.281 5.	-0.867 —4.973 O	-0.867	-0.501	0.356	0.248	Butyl acetate
Butanone 0.246 0.256 -0.080 -0.767 -4.855 0 4.148 5.	-0.767 —4.855 O	-0.767	-0.080		0.246	
Acetonitrile 0.413 0.077 0.326 -1.566 -4.391 0 3.364 5.						
Proprionitrile a 0.264 0.152 0.168 -1.427 -4.605 0 3.858 5						
Butyronitrile a 0.279 0.237 -0.053 -1.265 -4.629 0 3.978 5						
Wet octanol 0.088 0.562 -1.054 0.034 -3.460 0 3.814 4.						9
Gas - water - 0.994 0.577 2.549 3.813 4.841 0 - 0.869 2.						

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