Journal of Molecular Liquids 238 (2017) 58–61

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

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

Michael H. Abraham [a,*], William E. Acree Jr [b]

[a] Department of Chemistry, University College London, 20 Gordon St, London WC1H 0AJ, UK
[b] Department of Chemistry, 1155 Union Circle Drive #305070, University of North Texas, Denton, TX 76203-5017, USA

ARTICLE INFO

Article history:
Received 28 March 2017
Received in revised form 24 April 2017
Accepted 26 April 2017
Available online 27 April 2017

Keywords:
trans-Stilbene
Gas-solvent partition coefficients
Water-solvent partition coefficients
Quantitative structure-property relationships
Solubility
Linear free energy relationships
Hydrogen-bonding

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.

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.

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

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

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 $cm^3\ mol^{-1}/10$, **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 $cm^3\ mol^{-1}/100$ 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].

* Corresponding author.
E-mail addresses: m.h.abraham@ucl.ac.uk (M.H. Abraham), bill.acree@unt.edu (W.E. Acree).

http://dx.doi.org/10.1016/j.molliq.2017.04.119
0167-7322/

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*.

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

Table 2
Coefficients 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]

								Log *P*	
Solvent, Eq. (1)	*c*	*e*	*s*	*a*	*b*	*l*	*v*	Calc	Obs
Tetrachloromethane	0.199	0.523	−1.159	−3.560	−4.594	0	4.618	5.66	5.67
Hexane	0.333	0.560	−1.710	−3.578	−4.939	0	4.463	4.86	4.93
Heptane	0.297	0.634	−1.755	−3.571	−4.946	0	4.488	4.91	4.94
Octane	0.231	0.738	−1.840	−3.685	−4.907	0	4.502	4.91	4.95
Nonane	0.240	0.619	−1.713	−3.532	−4.921	0	4.482	4.87	4.96
Decane	0.186	0.722	−1.741	−3.449	−4.970	0	4.476	4.91	4.96
Hexadecane	0.087	0.667	−1.617	−3.587	−4.869	0	4.433	4.84	4.94
Cyclohexane	0.159	0.784	−1.678	−3.740	−4.929	0	4.577	5.21	5.17
Methylcyclohexane	0.246	0.782	−1.982	−3.517	−4.293	0	4.528	4.99	5.11
Cyclooctane a	−0.123	0.677	−1.697	−3.519	−5.568	0	5.026	5.31	5.26
t-Butylcyclohexane a	0.172	0.759	−2.025	−2.971	−4.663	0	4.655	4.95	5.02
Isooctane	0.318	0.555	−1.737	−3.677	−4.864	0	4.417	4.75	4.75
Squalane a	0.282	0.469	−1.303	−3.661	−5.126	0	4.107	4.58	4.75
Benzene	0.142	0.464	−0.588	−3.099	−4.625	0	4.491	6.01	5.89
Toluene	0.125	0.431	−0.644	−3.002	−4.748	0	4.524	5.91	5.81
m-Xylene	0.122	0.377	−0.603	−2.981	−4.961	0	4.535	5.85	5.75
p-Xylene	0.166	0.477	−0.812	−2.939	−4.874	0	4.532	5.79	5.77
Ethylbenzene	0.093	0.467	−0.723	−3.001	−4.844	0	4.514	5.79	5.70
Chlorobenzene	0.065	0.381	−0.521	−3.183	−4.700	0	4.614	6.08	5.91
Methanol	0.276	0.334	−0.714	0.243	−3.320	0	3.549	4.65	4.75
Ethanol	0.222	0.471	−1.035	0.326	−3.596	0	3.857	4.81	4.80
Propan-1-ol	0.139	0.405	−1.029	0.247	−3.767	0	3.986	4.80	4.80
Butan-1-ol	0.165	0.401	−1.011	0.056	−3.958	0	4.044	4.89	4.83
Pentan-1-ol	0.15	0.536	−1.229	0.141	−3.864	0	4.077	4.87	4.87
Hexan-1-ol	0.115	0.492	−1.164	0.054	−3.978	0	4.131	4.91	4.90
Heptan-1-ol	0.035	0.398	−1.063	0.002	−4.342	0	4.317	5.03	4.95
Octan-1-ol	−0.034	0.489	−1.044	−0.024	−4.235	0	4.218	4.98	4.97
Decan-1-ol	−0.058	0.616	−1.319	0.026	−4.153	0	4.279	4.91	4.96
Propan-2-ol	0.099	0.344	−1.049	0.406	−3.827	0	4.033	4.72	4.66
iso-Butanol	0.188	0.354	−1.127	0.016	−3.568	0	3.986	4.71	4.62
2-Butanol	0.127	0.253	−0.976	0.158	−3.882	0	4.114	4.82	4.68
t-Butanol	0.211	0.171	−0.947	0.331	−4.085	0	4.109	4.78	4.57
2-Methylbutan-2-ol	0.177	0.316	−1.125	0.306	−4.112	0	4.178	4.83	4.79
3-Methylbutan-1-ol	0.073	0.360	−1.273	0.090	−3.770	0	4.273	4.83	4.73
2-Pentanol	0.115	0.455	−1.331	0.206	−3.745	0	4.201	4.82	4.75
2-Methylpentan-1-ol	0.074	0.423	−1.228	0.143	−4.031	0	4.221	4.83	4.75
4-Methylpentan-2-ol	0.055	0.369	−1.340	0.211	−4.035	0	4.322	4.76	4.67
2-Ethylhexan-1-ol	0.061	0.459	−1.067	−0.178	−4.117	0	4.120	4.88	4.81
Cyclopentanol a	0.540	0.663	−1.172	−0.027	−3.387	0	3.600	4.86	5.03
Trifluoroethanol	0.395	−0.094	−0.594	−1.280	−1.274	0	3.088	4.08	4.03
Ethylene glycol	−0.270	0.578	−0.511	0.715	−2.619	0	2.729	3.55	3.79
Dibutylether	0.176	0.394	−0.985	−1.414	−5.357	0	4.524	5.35	5.28
Methyl t-butyl ether	0.341	0.307	−0.817	−0.618	−5.097	0	4.425	5.51	5.45
Tetrahydrofuran	0.207	0.372	−0.392	−0.236	−4.934	0	4.447	6.05	6.12
Dioxane	0.098	0.350	−0.083	−0.556	−4.826	0	4.172	5.88	5.93
Methyl acetate	0.351	0.223	−0.150	−1.035	−4.527	0	3.972	5.64	5.70
Ethyl acetate	0.328	0.369	−0.446	−0.700	−4.904	0	4.150	5.65	5.72
Butyl acetate	0.248	0.356	−0.501	−0.867	−4.973	0	4.281	5.67	5.69
Butanone	0.246	0.256	−0.080	−0.767	−4.855	0	4.148	5.86	5.89
Acetonitrile	0.413	0.077	0.326	−1.566	−4.391	0	3.364	5.16	5.33
Proprionitrile a	0.264	0.152	0.168	−1.427	−4.605	0	3.858	5.64	5.69
Butyronitrile a	0.279	0.237	−0.053	−1.265	−4.629	0	3.978	5.68	5.76
Wet octanol	0.088	0.562	−1.054	0.034	−3.460	0	3.814	4.74	4.81
Gas –water	−0.994	0.577	2.549	3.813	4.841	0	−0.869	2.62	2.52