Descriptors for Vitamin K3 (Menadione); calculation of biological and physicochemical properties

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ABSTRACT

We have used literature values for the solubility of vitamin K3 in organic solvents to obtain Abraham descriptors for vitamin K3. Although these descriptors themselves are not exceptional in any way, when combined with equations that we have already set out, they lead to the prediction of important properties of vitamin K3. These include the vapor pressure and heat of sublimation (necessary for the analysis of data on the concentration of vitamin K3 in ambient air), and the partitions air-water, air-blood, air-lung, air-fat, air-skin, water-lipid, water-membrane, water-skin, as well as permeation from water through skin. Values of the partitions into biological phases are all quite large by comparison to those for organic compounds in general.

Keywords: Vitamin K3, Menadione, 2-methyl-1,4-naphthoquinone, Abraham descriptors, solubility, linear free energy relationships, partitions

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1. Introduction

Vitamin K3 (VK3), also known as menadione (2-methyl-1,4-naphthoquinone) is a synthetic, artificially produced form of vitamin K that does not occur naturally, unlike the other two forms of vitamin K—vitamin K1 (VK1), known as phylloquinone, and vitamin K2 (VK2), called menaquinone. VK3 is an essential nutrient involved in blood clotting and bone health [1]. It has been known to have anticancer activity against various types of adult cancer cells [2, 3] compared to the natural compounds such as VK1 and VK2 [4]. It was found to be effective against cancers such as breast, bladder, hepatic, mammary, oral cavity, pharyngeal and blood cancers in vitro as well as parental and multidrug resistant leukaemia cell lines [5]. VK3 was reported to show anti-cancer mechanisms by producing reactive oxygen species (ROS), including hydroxyl radicals, superoxide radicals and hydrogen peroxide [6]. VK3 also demonstrated anti-bacterial effects [7-10]. It showed the antibiotic-modifying activity in multi-resistant strains of *Staphylococcus aureus*, *Pseudomonas aeruginosa*, and *Escherichia coli* [11]. It was suggested that VK3 potentiated aminoglycosides against multi-resistant bacteria since it lowered the minimal inhibitory concentration (MIC) of the antibiotics [11].

Biproducts in the synthesis of VK3 include phthalic anhydride, 2-naphthaldehyde and 6-methyl-1,4-naphthoquinone, and separation of VK3 from byproducts is a key step in its manufacture. A knowledge of the solubility of VK3 in solvents is of considerable help in the design of separation processes. To date the solubility of VK3 is known at 298 K in ten aliphatic solvents [12], and six aromatic hydrocarbons [13], and at only one point (wt % water = 0.60) in a number of water-solvent mixtures [14]. We aim to correlate the solubility of VK3 in the sets of pure solvents [12, 13], with Abraham parameters, and then to enable predictions of solubilities in a very large number of non-aqueous solvents and water-solvent mixtures to be made. We can then use the obtained Abraham parameters for VK3 to predict other important physicochemical and biological properties of VK3.

2. Methods

We have constructed two general linear free energy relationships, LFERs, Equations (1) and (2), that can be used to analyze the transfer of neutral solutes from water to organic solvents and from the gas phase to organic solvents. The dependent variables in Equation (1) and Equation (2) are log *P*, where *P* is the molar water to solvent partition coefficient for a series of solutes, and log *K* where *K* is the dimensionless gas phase to solvent partition coefficient for a series of solutes.

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

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

The independent variables, or descriptors, in Equations (1) and (2) are properties of the neutral solutes as follows [15-21]. *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. We give the coefficients in Equations (1) and (2) for systems that we consider here are shown in Table 1.

E is obtained from the refractive index of liquid compounds at 293 K [15] and for gases and solids the refractive index can be estimated [22] or *E* itself can be calculated[23] [24]. The descriptors *S, A, B* and *L* can be obtained from water to solvent partition measurements [20, 22], and from solubilities in nonaqueous sovents, C_S [17, 21]. The latter can be transformed into water-solvent partition coefficients through Equation (3), where C_W is the corresponding solubility in water [17, 20-22, 25]. If an experimental value of log *Cw* is not available, it can be added as another unknown descriptor to be determined.

$$P = C_S / C_W \qquad \log P = \log C_S - \log C_W \quad (3)$$

Finally, values of *P* can be converted into the air-solvent partition coefficient *K* through Equation (4) [25].

$$\log K - \log Kw = \log P \quad (4)$$

where *Kw* is the dimensionless air to water partition coefficient defined through equation (5); C_W and the corresponding gaseous concentration, C_G, are in units of mol dm^{-3} [25].

$$Kw = C_W / C_G \quad (5)$$

Table 1.

Coefficients in Equations (1) and (2); calculated and observed values of log *P* and log *K* for transfer of Vitamin K3 from water and from the gas phase to solvents at 298 K

Solvent	***c***	***e***	***s***	***a***	***b***	***l***	***v***		**Calc**	**Obs**
Dichloromethane	0.319	0.102	-0.187	-3.058	-4.090	0.000	4.324	Log P	3.585	3.521
1,2-Dichloroethane	0.183	0.294	-0.134	-2.801	-4.291	0.000	4.180	Log P	3.472	3.377
Cyclohexane	0.159	0.784	-1.678	-3.740	-4.929	0.000	4.577	Log P	1.947	1.912
Benzene	0.142	0.464	-0.588	-3.099	-4.625	0.000	4.491	Log P	3.196	3.140
Toluene	0.125	0.431	-0.644	-3.002	-4.748	0.000	4.524	Log P	3.031	3.069
o-Xylene	0.083	0.518	-0.813	-2.884	-4.821	0.000	4.559	Log P	2.854	3.102
m-Xylene	0.122	0.377	-0.603	-2.981	-4.961	0.000	4.535	Log P	2.921	3.061
p-Xylene	0.166	0.477	-0.812	-2.939	-4.874	0.000	4.532	Log P	2.823	3.056
Ethylbenzene	0.093	0.467	-0.723	-3.001	-4.844	0.000	4.514	Log P	2.862	2.932
Methyl acetate	0.351	0.223	-0.150	-1.035	-4.527	0000	3.972	Log P	3.130	3.107
Propanone	0.313	0.312	-0.121	-0.608	-4.753	0.000	3.942	Log P	3.085	3.027
Acetonitrile	0.413	0.077	0.326	-1.566	-4.391	0.000	3.364	Log P	2.996	2.953
Methanol	0.276	0.334	-0.714	0.243	-3.320	0.000	3.549	Log P	2.460	2.285
Propan-1-ol	0.139	0.405	-1.029	0.247	-3.767	0.000	3.986	Log P	2.273	2.164
Butan-1-ol	0.165	0.401	-1.011	0.056	-3.958	0.000	4.044	Log P	2.293	2.152
Propan-2-ol	0.099	0.344	-1.049	0.406	-3.827	0.000	4.033	Log P	2.156	2.115
Wet octan-1-ol	0.088	0.562	-1.054	0.034	-3.460	0.000	3.814	Log P	2.323	2.210
Gas-water	-0.994	0.577	2.549	3.813	4.841	0.000	-0.869	Log Kw	4.984	5.038
Dichloromethane	0.192	-0.572	1.492	0.460	0.847	0.965	0.000	Log K	8.672	8.559
1,2-Dichloroethane	0.017	-0.337	1.600	0.724	0.000	1.016	0.000	Log K	8.539	8.415
Cyclohexane	0.163	-0.110	0.000	0.000	0.000	1.013	0.000	Log K	6.880	6.950
Benzene	0.107	-0.313	1.053	0.457	0.169	1.020	0.000	Log K	8.267	8.178
Toluene	0.085	-0.400	1.063	0.501	0.154	1.011	0.000	Log K	8.082	8.107
o-Xylene	0.064	-0.296	0.934	0.647	0.000	1.010	0.000	Log K	7.910	8.140
m-Xylene	0.071	-0.423	1.068	0.552	0.000	1.014	0.000	Log K	7.984	8.099
p-Xylene	0.113	-0.302	0.826	0.651	0.000	1.011	0.000	Log K	7.799	8.094
Ethylbenzene	0.059	-0.295	0.924	0.573	0.098	1.010	0.000	Log K	7.945	7.970
Methyl acetate	0.134	-0.477	1.749	2.678	0.000	0.876	0.000	Log K	8.053	8.145
Propanone	0.127	-0.387	1.733	3.060	0.000	0.866	0.000	Log K	8.068	8.065
Acetonitrile	-0.007	-0.595	2.461	2.085	0.418	0.738	0.000	Log K	8.111	7.991
Methanol	-0.039	-0.338	1.317	3.826	1.396	0.773	0.000	Log K	7.472	7.323
Propan-1-ol	-0.042	-0.246	0.749	3.888	1.076	0.874	0.000	log K	7.254	7.202
Butan-1-ol	-0.004	-0.285	0.768	3.705	0.879	0.890	0.000	log K	7.273	7.190
Propan-2-ol	-0.048	-0.324	0.713	4.036	1.055	0.884	0.000	log K	7.153	7.153
Wet octan-1-ol	-0.222	0.088	0.701	3.473	1.477	0.851	0.000	Log K	7.481	7.248
Gas-water	-1.271	0.822	2.743	3.904	4.814	-0.213	0.000	Log Kw	4.974	5.038
GLC-NIST	0.070	0.012	0.076	0.000	0.000	0.200	0.000	I/1000	1.551	1.581

3. Results and Discussion

The values of log *P* and log *K* that we have obtained from the observed solubilities of VK3 are in Table 1, together with values of log *Kw* and a gas-chromatographic retention index [26]. These yield no less than 37 simultaneous equations of the form of Equations (1) and (2) that can be solved to yield values of the descriptors. It is useful to be able to reduce the number of descriptors that have to be determined. *E* was set as 1.25 from a calculated refractive index [22], and *V* calculated as 1.3007, trivially [15]. This left *S, A, B, L,* log *Kw* and log *Cw* to be determined. With the obtained descriptors in Table 2, the 37 equations were solved with a standard deviation in observed and calculated dependent variables of only 0.124 log units. Our calculated aqueous solubility of log *Cw* = -3.124 with *Cw* in units of mol dm $^{-3}$ at 298 K is in excellent agreement with an experimental value of -3.05 at 306 K [27], and our calculated water-octanol partition coefficient, as log *P* = 2.32 (Table 1) is in good agreement with the experimental value of 2.21 [28].

Now that we have descriptors for VK3, we can use equations on the lines of Equations (1) and (2) to predict values of the dependent variables for a very large number of systems. Thus we can predict log *Cs* and hence log *P* for some 100 dry solvents [29-34], some 100 wet solvents [29, 30, 35] and slightly more than 90 ionic liquids [36] [37] [38] [39] [40] [41] at 298 K. We have also developed an ion-specific equation coefficient version of the Abraham model that allows one to construct predictive log *K* and log *P* equations by generating the each equation coefficients as an individual cation plus anion sum [42-44]. The 67-cation-specific and 20 anion-specific equation coefficients that we have determined to date can be combined to give predictive log *K* and log *P* expressions for 1340 (67x20) different ionic liquids. Each of the predictive expressions does require a prior knowledge of the solute descriptor values for the compound whose partition coefficients and solubilities are being predicted.

Delgado-Saborit et al. [45] have shown that VK3 is present in ambient air. They correlated concentrations in ambient air of a set of compounds against their vapor pressure and Henry's constant, but were not able to include VK3 because of lack of data. We have obtained equations for the thermodynamics of sublimation of organic solids, and can use these to predict the vapor pressure [46] log(VP/atm), the enthalpy of sublimation [47] *Hsub*/kJ mol $^{-1}$ and the heat capacity of sublimation [48] $\Delta_{sub}Cp$ /J K^{-1} mol $^{-1}$, all at 298 K. The latter two quantities can be used to predict the vapor pressure at other temperatures. Our predictions at 298 K are in Table 3.

Since VK3 can be found in ambient air [45] and then partition into water, partitions of VK3 between air and physical or biological phases and between water and biological phases become important. We have set out equations on the lines of Equation (2) for air to a number of biological phases at 310 K [49, 50], and give the most relevant predictions in Table 3. The air to biological phase predicted values are all very large by comparison to organic compounds in general.

Endo et al. [51] have obtained coefficients in Equation (1) for several processes of environmental importance and we have used these to make a number of useful predictions, see Table 3. These predicted values are not unusual and fall in the middle of the experimental range of values for other organic compounds. We can also use our equation [52] to calculate the skin permeation from water for VK3. Our value of log kp (cm s^{-1}) = -5.02 is a little higher that the average for a set of compounds, -6.0, so that VK3 permeates rather faster than the average organic chemical.

The predicted values in Table 3 are all 'outright' predictions. No previous data on VK3 was used in any way, and to our knowledge there is no literature data on VK3 for any of the systems in Table 3.

Table 2

Descriptors for VK3 obtained by solution of the 37 simultaneous equations

E	***S***	***A***	***B***	***V***	***L***	**Log *Kw***	**Log *Cw***
1.25	1.48	0.00	0.54	1.3007	6.766	5.04	-3.124

Table 3

Predictions of thermodynamic and biological properties of VK3

Process	**Detail**	**T/K**	**Value**	**Equation**	**Ref**
Vapor pressure	Log(VP/atm)	298	-6.33	Eqn in V	[46]
Vapor pressure	Log(VP/atm)	298	-6.57	Eqn in L	[46]
Enthalpy of sublimation	*Hsub*/kJ mol^{-1}	298	93.9	Eqn. in V	[47]

Enthalpy of sublimation	*Hsub*/kJ mol^{-1}	298	96.9	Eqn. in L	[47]
Heat capacity of sublimation	$\Delta_{sub}Cp$/ J K^{-1} mol^{-1}	298	-36.6	Eqn in V	[48]
Heat capacity of sublimation	$\Delta_{sub}Cp$/ J K^{-1} mol^{-1}	298	-37.9	Eqn in L	[48]
Air to brain	Log*(Cbrain/Cair)*	310	5.04	Eqn in L	[49] [50]
Air to blood	Log*(Cblood/Cair)*	310	5.01	Eqn in L	[49] [50]
Air to lung	Log*(Clung/Cair)*	310	5.57	Eqn in L	[49] [50]
Air to fat (lipid)	Log*(Cfat/Cair)*	310	6.30	Eqn in L	[49] [50]
Air to water	Log*(Cwater/Cair)*	310	4.55	Eqn in L	[49] [50]
Air to skin	Log*(Cskin/Cair)*	310	6.66	Eqn. in L	[49] [50]
Water to storage lipid	Log*(Clipid/Cwater)*	310	2.32	Eqn. in V	[51]
Water to membrane	Log*(Cmem/Cwater)*	310	2.48	Eqn. in V	[51]
Water to bovine serum albumin	Log*(Calbum/Cwater)*	310	2.28	Eqn. in V	[51]
Water to muscle protein	Log*(Cmuscle/Cwater)*	310	1.54	Eqn. in V	[51]
Water to (wet) skin	Log*(Cskin/Cwater)*	310	1.63	Eqn. in V	[49], [50]
Skin permeation from water	Log (kp in cm s^{-1})	310	-5.02	Eqn. in V	[52]

4. Conclusions

Solubility data for vitamin K3 can be used to obtain Abraham descriptors with good agreement between observed and calculated solubilities as shown in Table 1. The descriptors themselves are not exceptional but they are valuable in that together with equations we have already constructed they lead to the prediction of values of vitamin K3 in large number of important physicochemical and biological processes, none of which have been investigated previously.

Conflicts of Interest

There are no conflicts of interest to declare

References

[1] S. Akbari, A.A. Rasouli-Ghahroudi, Vitamin K and Bone Metabolism: A Review of the Latest Evidence in Preclinical Studies, Biomed Res Int 2018 (2018) 4629383.
[2] F.Y. Wu, T.P. Sun, Vitamin K3 induces cell cycle arrest and cell death by inhibiting Cdc25 phosphatase, Eur J Cancer 35(9) (1999) 1388-93.
[3] L.M. Nutter, A.L. Cheng, H.L. Hung, R.K. Hsieh, E.O. Ngo, T.W. Liu, Menadione: spectrum of anticancer activity and effects on nucleotide metabolism in human neoplastic cell lines, Biochem Pharmacol 41(9) (1991) 1283-92.
[4] R. Sasaki, Y. Suzuki, Y. Yonezawa, Y. Ota, Y. Okamoto, Y. Demizu, P. Huang, H. Yoshida, K. Sugimura, Y. Mizushina, DNA polymerase gamma inhibition by vitamin K3 induces mitochondria-mediated cytotoxicity in human cancer cells, Cancer Sci 99(5) (2008) 1040-8.
[5] K.W. Wellington, V. Hlatshwayo, N.I. Kolesnikova, S.T. Saha, M. Kaur, L.R. Motadi, Anticancer activities of vitamin K3 analogues, Invest New Drugs 38(2) (2020) 378-391.
[6] M. Tomasetti, E. Strafella, S. Staffolani, L. Santarelli, J. Neuzil, R. Guerrieri, alpha-Tocopheryl succinate promotes selective cell death induced by vitamin K3 in combination with ascorbate, Br J Cancer 102(8) (2010) 1224-34.
[7] D. Dey, R. Ray, B. Hazra, Antitubercular and antibacterial activity of quinonoid natural products against multi-drug resistant clinical isolates, Phytother Res 28(7) (2014) 1014-21.
[8] B.S. Park, H.K. Lee, S.E. Lee, X.L. Piao, G.R. Takeoka, R.Y. Wong, Y.J. Ahn, J.H. Kim, Antibacterial activity of Tabebuia impetiginosa Martius ex DC (Taheebo) against Helicobacter pylori, J Ethnopharmacol 105(1-2) (2006) 255-62.
[9] P.M. Schlievert, J.A. Merriman, W. Salgado-Pabon, E.A. Mueller, A.R. Spaulding, B.G. Vu, O.N. Chuang-Smith, P.L. Kohler, J.R. Kirby, Menaquinone analogs inhibit growth of bacterial pathogens, Antimicrob Agents Chemother 57(11) (2013) 5432-7.
[10] T. Sreelatha, S. Kandhasamy, R. Dinesh, S. Shruthy, S. Shweta, D. Mukesh, D. Karunagaran, R. Balaji, N. Mathivanan, P.T. Perumal, Synthesis and SAR study of novel anticancer and antimicrobial naphthoquinone amide derivatives, Bioorg Med Chem Lett 24(15) (2014) 3647-51.
[11] J.C. Andrade, M.F. Morais Braga, G.M. Guedes, S.R. Tintino, M.A. Freitas, L.J. Quintans, Jr., I.R. Menezes, H.D. Coutinho, Menadione (vitamin K) enhances the antibiotic activity of drugs by cell membrane permeabilization mechanism, Saudi J Biol Sci 24(1) (2017) 59-64.
[12] Y. Yu, F. Li, S. Long, L. Xu, G. Liu, Solubility, thermodynamic properties, HSP, and molecular interactions of vitamin K3 in pure solvents, Journal of Molecular Liquids 317 (2020) 113945.
[13] C.Y. Song, H.Z. Shen, L.C. Wang, J.H. Zhao, F.A. Wang, Solubilities of Vitamin K3 in benzene, toluene, ethylbenzene, o-xylene, m-xylene and p-xylene between (299,44 and 344.24) K, J. Chem. Eng. Data 53 (2008) 283-285.
[14] C.Y. Song, H.Z. Shen, J.H. Zhao, L.C. Wang, F.A. Wang, Solubilities of 2-methyl-1,4-naphthoquinone in water + (methanol, ethanol, 1-propanol, 2-propanol, 1,2-propanediol and glycerine, respectively) from (293.15 to 337.92) K, **J. Chem. Eng. Data** 52 (**2007**).
[15] M.H. Abraham, Scales of Solute Hydrogen-Bonding - Their Construction and Application to Physicochemical and Biochemical Processes, Chem Soc Rev 22(2) (1993) 73-83.
[16] M.H. Abraham, A. Ibrahim, A.M. Zissimos, Determination of sets of solute descriptors from chromatographic measurements, J Chromatogr A 1037(1-2) (2004) 29-47.
[17] M.H. Abraham, J.W.E. Acree, M. Brumfield, E. Hart, L. Pipersburgh, K. Mateja, C. Dai, D.I. Grover, S. Zhang, The deduction of physicochemical properties from solubilities; 2,4-

dihydroxybenzophenone, biotin and caprolactam as examples, J. Chem. Eng. Data 60 (2015) 1440-1446.
[18] C.F. Poole, T.C. Ariyasena, N. Lenca, Estimation of the environmental properties of compounds from chromatographic measurements and the solvation parameter model, Journal of Chromatography A 1317 (2013) 85-104.
[19] C.F. Poole, S.N. Atapattu, S.K. Poole, A.K. Bell, Determination of solute descriptors by chromatographic methods, Anal Chim Acta 652(1-2) (2009) 32-53.
[20] E.D. Clarke, L. Mallon, The Determination of Abraham descriptors and their Application to Crop Protection Research, in: P. Jeschke, W. Krämer, U. Schirmer, M. Witschel (Eds.), Modern Methods in Crop Protection Research, Wiley-VCH Verlag GmbH & Co2012.
[21] M.H. Abraham, R.E. Smith, R. Luchtefeld, A.J. Boorem, R. Luo, W.E. Acree, Jr., Prediction of solubility of drugs and other compounds in organic solvents, J Pharm Sci 99(3) (2010) 1500-15.
[22] A.C.D. ChemSketch, 110 Yonge Street, 14th Floor, Toronto, Ontario, M5C 1T4, Canada.
[23] N. Ulrich, S. Endo, T.N. Brown, N. Watanabe, G. Bronner, M.H. Abraham, K.U. Goss, UFZ-LSER database v 3.2.1 Leipzig, Germany, Helmholtz Centre for Environmental Research-UFZ, 2017.
[24] v. ADME, Advanced Chemistry Development, 110 Yonge Street, 14th Floor, Toronto, Ontario, M5C 1T4, Canada.
[25] M.H. Abraham, W.E. Acree, D. Hoekman, A.J. Leo, M.L. Medlin, A new method for the determination of Henry's law constants (air-water-partition coefficients), Fluid Phase Equilibr 502 (2019).
[26] NIST.
[27] M.D. Dubbs, R.B. Gupta, Solubility of Vitamin E (-Tocophenol) and Vitamin K3 (Menadione) in Ethanol-Water mixtures. , J. Chem. Eng. Data 43 (1998) 590-591.
[28] BioLoom, BioByte Corp, 201 W. 4th Street, #204 Claremont, CA 91711-4707, USA.
[29] M.H. Abraham, W.E. Acree, Gas-solvent and water-solvent partition of trans-stilbene at 298 K, Journal of Molecular Liquids 238 (2017) 58-61.
[30] M.H. Abraham, W.E. Acree, Descriptors for ferrocene and some substituted ferrocenes, Journal of Molecular Liquids 232 (2017) 325-331.
[31] I.A. Sedov, D. Khaibrakhmanova, E. Hart, D. Grover, H. Zettl, V. Koshevarova, C. Dai, S.S.N. Zhang, A. Schmidt, W.E. Acree, M.H. Abraham, Development of Abraham model correlations for solute transfer into both 2-propoxyethanol and 2-isopropoxyethanol at 298.15 K, Journal of Molecular Liquids 212 (2015) 833-840.
[32] E. Hart, D. Grover, H. Zettl, V. Koshevarova, S. Zhang, C. Dai, W.E. Acree, I.A. Sedov, M.A. Stolov, M.H. Abraham, Abraham model correlations for solute transfer into 2-methoxyethanol from water and from the gas phase, Journal of Molecular Liquids 209 (2015) 738-744.
[33] E. Hart, A. Klein, M. Barrera, M. Jodray, K. Rodriguez, W.E.J. Acree, M.H. Abraham, Development of Abraham model correlations for describing the transfer of molecular solutes into propanenitril and butanenitrile from water and from the gas phase, Phys. Chem. Liq 56 (2018) 821-833.
[34] M.H. Abraham, M. Zad, W.E. Acree, The transfer of neutral molecules from water and from the gas phase to solvents acetophenone and aniline, Journal of Molecular Liquids 212 (2015) 301-306.
[35] B. Churchill, W.E. Acree, M.H. Abraham, Abraham model correlation for direct water-to-2,2,5,5-tetramethyloxolane solute transfer partitioning process revisited, Phys Chem Liq (2019).

[36] B.H. Jiang, M.Y. Horton, W.E. Acree, M.H. Abraham, Ion-specific equation coefficient version of the Abraham model for ionic liquid solvents: determination of coefficients for tributylethylphosphonium, 1-butyl-1-methylmorpholinium, 1-allyl-3-methylimidazolium and octyltriethylammonium cations, Phys Chem Liq 55(3) (2017) 358-385.
[37] F. Mutelet, G.A. Baker, H. Zhao, B. Churchill, W.E.J. Acree, Development of Abraham model correlations for short-chain glycol-grafted imidazolium and pyridinium ionic liquids from inverse gas-chromatographic measurements, J. Mol. Liq 317 (2020) 113983/1-113983/12.
[38] F. Mutelet, C. Hussard, G.A. Baker, H. Zhao, B. Churchill, W.E. Acree, Characterization of the solubilizing ability of short-chained glycol-grafted ammonium and phosphonium ionic liquids, Journal of Molecular Liquids 304 (2020).
[39] F. Rabhi, F. Mutelet, H. Sifaoui, D.V. Wagle, G.A. Baker, B. Churchill, W.E. Acree, Characterization of the solubilizing ability of tetraalkylammonium ionic liquids containing a pendant alkyl chain bearing a basic N,N-dimethylamino or N,N-dimethylaminoethoxy functionality, Journal of Molecular Liquids 283 (2019) 380-390.
[40] F. Mutelet, G.A. Baker, S. Ravula, E. Qian, L. Wang, W.E. Acree, Infinite dilution activity coefficients and gas-to-liquid partition coefficients of organic solutes dissolved in 1-sec-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide and in 1-tert-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, Phys Chem Liq 57(4) (2019) 453-472.
[41] F. Mutelet, S. Ravula, G.A. Baker, D. Woods, X. Tong, W. Acree, Infinite Dilution Activity Coefficients and Gas-to-Liquid Partition Coefficients of Organic Solutes Dissolved in 1-Benzylpyridinium Bis(Trifluoromethylsulfonyl)Imide and 1-Cyclohexylmethyl-1-Methylpyrrolidinium Bis(Trifluoromethylsulfonyl)Imide, J Solution Chem 47(2) (2018) 308-335.
[42] L. Sprunger, M. Clark, W.E. Acree, M.H. Abraham, Characterization of room-temperature ionic liquids by the abraham model with cation-specific and anion-specific equation coefficients, J Chem Inf Model 47(3) (2007) 1123-1129.
[43] L.M. Sprunger, A. Proctor, W.E.J. Acree, M.H. Abraham, LFER correlations for room temperature ionic liquids: Separation of equation coeffi cients into individual cation-specific and anion-specific contributions, Fluid Phase Equilib 265 (2008) 104-111.
[44] T.W. Stephens, V. Chou, A.N. Quay, C. Shen, N. Dabadge, A. Tian, M. Loera, B. Willis, A. Wilson, W.E. Acree, P. Twu, J.L. Anderson, M.H. Abraham, Thermochemical investigations of solute transfer into ionic liquid solvents: updated Abraham model equation coefficients for solute activity coefficient and partition coefficient predictions, Phys Chem Liq 52(4) (2014) 488-518.
[45] J.M. Delgado-Saborit, M.S. Alam, K.J.G. Pollitt, C. Stark, R.M. Harrison, Analysis of atmospheric concentrations of quinones and polycyclic aromatic hydrocarbons in vapour and particulate phases, Atmos Environ 77 (2013) 974-982.
[46] M.H. Abraham, W.E.J. Acree, Estimation of vapor pressures of liquid and solid organic and organometallic compounds at 298.15K, Fluid Phase Equilib 519 (2020) 112595.
[47] M.H. Abraham, W.E. Acree, Estimation of enthalpies of sublimation of organic, organometallic and inorganic compounds, Fluid Phase Equilibr 515 (2020).
[48] M.H. Abraham, W.E.J. Acree, Estimation of heat capacities of gases, liquids and solids, and heat capacities of vaporization and of sublimation of organic chemicals at 298.15 K, J. Mol. Liquids 515 (2020) 112575.
[49] M.H. Abraham, J.M.R. Gola, A. Ibrahim, W.E. Acree, X.L. Liu, The prediction of blood-tissue partitions, water-skin partitions and skin permeation for agrochemicals, Pest Manag Sci 70(7) (2014) 1130-1137.

[50] M.H. Abraham, J.M. Gola, A. Ibrahim, W.E. Acree, Jr., X. Liu, A simple method for estimating in vitro air-tissue and in vivo blood-tissue partition coefficients, Chemosphere 120 (2015) 188-91.
[51] S. Endo, T.N. Brown, K.U. Goss, General Model for Estimating Partition Coefficients to Organisms and Their Tissues Using the Biological Compositions and Polyparameter Linear Free Energy Relationships, Environmental Science & Technology 47(12) (2013) 6630-6639.
[52] K.D. Zhang, M.H. Abraham, X.L. Liu, An equation for the prediction of human skin permeability of neutral molecules, ions and ionic species, Int J Pharmaceut 521(1-2) (2017) 259-266.