Pharmaceutical Sciences
June 2019, 25(2), 165-170
doi: 10.15171/PS.2019.24
https://ps.tbzmed.ac.ir/

Short Communication

Further Analysis on Solubility Measurement and Thermodynamic Modeling of Benzoic Acid in Monosolvents and Binary Mixtures

Abolghasem Jouyban[1,2], Elaheh Rahimpour[3], William E. Acree Jr.[4*]

[1]*Pharmaceutical Analysis Research Center and Faculty of Pharmacy, Tabriz University of Medical Sciences, Tabriz, Iran.*
[2]*Kimia Idea Pardaz Azarbayjan (KIPA) Science Based Company, Tabriz University of Medical Sciences, Tabriz, Iran.*
[3]*Food and Drug Safety Research Center, Tabriz University of Medical Sciences, Tabriz, Iran.*
[4]*Department of Chemistry, University of North Texas, Denton, TX 76203-5070, USA.*

Article Info

Article History:
Received: 25 November 2018
Revised: 18 December 2018
Accepted: 18 December 2018
ePublished: 30 June 2019

Keywords:
-Benzoic acid
-Solubility prediction
-Binary solvent mixtures

ABSTRACT

Background: Recently Sandeepa et al. reported the solubility of benzoic acid in six monosolvents (i.e. tributyl phosphate, diacetone alcohol, methyl-n-propyl ketone, methyl acetate, amyl acetate, and isooctane) and five binary systems (i.e. ethanol + hexane, isopropyl alcohol + hexane and chloroform + hexane, acetone + hexane, and acetone + water) along with some numerical analyses. The reported calculations have been reanalyzed and some recommendations and further computations were proposed.
Methods: Further analyses were performed based on combined nearly ideal binary solvent/Redlich-Kister, the modified Wilson model, general single model, Jouyban–Acree model and Jouyban–Acree–van't Hoff model.
Results: The mentioned numerical analyses were used to predict the solubility of benzoic acid in the binary solvent mixtures at various temperatures and the predicted solubility data were compared with their corresponding experimental values by calculating relative deviations.
Conclusion: The investigated models provide good estimation of the solubility behavior of benzoic acid in the binary solvent mixtures at various temperatures.

Introduction

In a recently published paper, Sandeepa *et al.*[1] reported the experimental solubility of benzoic acid in a number of mono-solvents including tributyl phosphate, diacetone alcohol, methyl-n-propyl ketone, methyl acetate, amyl acetate, and isooctane and five binary solvent systems (i.e. ethanol + hexane, isopropyl alcohol + hexane and chloroform + hexane, acetone + hexane, and acetone + water) at various temperatures along with some numerical analyses. Benzoic acid is used as an antimicrobial food additive to prevent the proliferation of bacteria, yeasts and moulds.[2] Benzoic acid was used as an expectorant, analgesic, and antiseptic in the early 20th century.[3] It can be used for the treatment of fungal skin diseases such as tinea, ringworm, and athlete's foot.[4] Benzoic acid is an important precursor for the industrial synthesis of many other organic substances. Therefore, its solubility determination and prediction in neat solvents or mixed systems can be useful for separation and purification of benzoic acid from reaction media. The generated experimental solubility data extends the solubility database of benzoic acid in mono-solvents and the mixed solvents and could be helpful in the pharmaceutical and chemical industries. In addition to experimental efforts, various numerical models proposed for the estimation of the solubility of drug and/or drug like compounds[5] in the mono-solvents and the cosolvency systems include the van't Hoff equation, Apelblat, and Buchowski (λh) models, the mixture response surface, the phenomenological model, the non-random two-liquid model (NRTL) model, the combined nearly ideal binary solvent/Redlich-Kister equation, the modified Wilson model, fluctuation theory, and the Jouyban-Acree model. Sandeepa *et al.*[1] correlated the experimental solubility data of benzoic acid in the binary solvent mixtures using the ʎh equation, the NRTL model, and the modified Apelblat−Jouyban−Acree model for aqueous binary solvent mixtures. Further analyses were performed in this study which provide more information for better understanding of the solubility behavior of benzoic acid in the investigated solvents.

Results and Discussion

At first, the reported calculations on solubility data of benzoic acid were reanalyzed. Sandeepa *et al.*[1] have correlated the mole fraction solubility data of benzoic acid in binary solvent systems at different temperatures with the ʎh equation expressed as:

$$x = \frac{\lambda}{e^{\lambda h(T^{-1}-T_m^{-1})} - 1 + \lambda} \qquad \text{Eq. (1)}$$

where x is the mole fraction solubility at temperature T;

***Corresponding Author**: William E. Acree Jr, E-mail: acree@unt.edu

T_m is the melting point of the solute. λ and h are the coefficients of model.

The accuracy of the computations were assessed using the relative deviation (*RD*) defined as

$$RD = \frac{1}{N}\sum\left(\frac{\left|x^{\text{exp.}} - x^{\text{cal.}}\right|}{x^{\text{exp.}}}\right) \quad \text{Eq. (2)}$$

and root mean square deviation (*RMSD*) as

$$RMSD = \sqrt{\frac{\sum (x^{\text{exp.}} - x^{\text{cal.}})^2}{N}} \quad \text{Eq. (3)}$$

where N is the number of experimental points, $x^{cal.}$ is the calculated solubility and $x^{\text{exp.}}$ is the experimental solubility.

The recalculated parameters for Eq. 1 by SPSS software version 16.0,[6] show an inconsistency for constants and *RD* obtained for all investigated systems. A comparison between reported data (Table 5 of the published paper) and our recalculated data is summarized in Table 1. However, the aim of this short communication is not to criticize valuable work of Sandeepa *et al.*, but rather is to report further calculations and to provide predictive computations.

Table 1. Recalculated parameters of the λh equation (Eq. 4 of the published paper) for describing the solubility of benzoic acid in ethanol (1) + hexane (2) solvent mixtures.

w_a[1]	Parameters (Table 5 Ref#1)			Parameters (recalculated data)		
	λ	*h*	*100RD*	*λ*	*h*	*100RD*
0.200	1.33	2755.10	1.26	0.732	1309	7.98
0.360	1.99	1796.16	2.06	0.920	2136	2.65
0.491	1.53	1975.27	0.81	0.941	2118	1.74
0.600	1.19	2135.63	0.79	0.968	2149	0.63
0.693	1.22	2027.23	1.29	0.950	1965	0.94
0.772	0.81	2349.37	1.51	0.847	1355	1.31
0.840	0.64	2509.70	0.80	0.832	1240	1.36
0.900	0.63	2485.36	1.02	0.829	1200	0.80

[1]w_a is the mole fraction of ethanol in the mixtures with water in the absence of solute.

In addition to the correlative models employed by Sandeepa et al.,[1] one may use the combined nearly ideal binary solvent/Redlich-Kister (CNIBS/R-K),[7] the modified Wilson[8] and general single models (GSM).[9] The models are

$$\ln x_m = w_1 \ln(x_1)_B + w_2 \ln(x_1)_C + w_1 w_2 \sum_{i=0}^{2} J_i (w_1 - w_2)^i \quad \text{Eq. (4)}$$

$$-\ln x_m^{sat} = 1 - \frac{w_1[1+\ln(x_1)]}{w_1 + w_2\lambda_{12}} - \frac{w_2[1+\ln(x_2)]}{w_1\lambda_{21} + w_2} \quad \text{Eq. (5)}$$

$$\ln x_m = B_0 + B_1 x_b + B_2 (x_b)^2 + B_3 (x_b)^3 + B_4 (x_b)^4 \quad \text{Eq. (6)}$$

The CNIBS/R-K, modified Wilson model and GSM are correlative models and produce the similar accuracies for a given solute in a certain binary solvent mixture at a constant temperature. We recommend to use the extended version (i.e. the Jouyban–Acree model and/or its combined version with the van't Hoff equation), which consider both solvent composition and temperature. The Jouyban-Acree model is one such versatile model with good predictability power over broad temperature range and solvent composition.[10-12] The general version of the Jouyban-Acree model is:

$$\ln x_{m,T}^{sat} = w_1 . \ln x_{1,T}^{sat} + w_2 . \ln x_{2,T}^{sat} + \frac{w_1 . w_2}{T} \sum_{i=0}^{2} J_i . (w_1 - w_2)^i \quad \text{Eq. (7)}$$

which correlates the solute solubility in binary solvent mixtures at various temperatures employing experimental solubility data in the mono-solvents. To cover this limitation, one may combine the model with van't Hoff equation as[13,14]

$$\ln x_{m,T}^{sat} = w_1 (A_1 + \frac{B_1}{T}) + w_2 (A_2 + \frac{B_2}{T}) + \frac{w_1 . w_2}{T} \sum_{i=0}^{2} J_i . (w_1 - w_2)^i \quad \text{Eq. (8)}$$

where $X_{m,T}^{sat}$ is the mole fraction solubility of solute (benzoic acid in this case) in the solvent mixtures at temperature T/K, w_1 and w_2 are the mass fractions of mono solvents 1 and 2, in the absence of the solute, and A_1, B_1, A_2, B_2 and J_i are constants of the model obtained by a regression analysis.

The experimental solubility results for benzoic acid in the investigated cosolvency systems are fitted to Eqs. 4 to 8 and the applied model constants are presented in Tables 2 to 5. The solubility of benzoic acid in the each system was back-calculated on the basis of the regressed values of the model parameters. The obtained values of the *100RD* are also tabulated in Tables 2 to 5. Using these computations, the solubility at each given temperature could be calculated in the acceptable error range in pharmaceutical and industrial applications by CNIBS/R-K model, modified Wilson model, GSM, Jouyban–Acree model and Jouyban-Acree-van't Hoff model.

By incorporating the structural information about the solute and solvents in the computations, a significant improvement may be achieved for the solubility prediction of drugs in the cosolvency systems as shown in an earlier work.[15] The basic quantitative structure property relationship (QSPR) is:[16]

$$J_i = J_{1,i}[(c_1 - c_2)^2] + J_{2,i}[E(e_1 - e_2)^2] + J_{3,i}[S(s_1 - s_2)^2] + J_{4,i}[A(a_1 - a_2)^2] + J_{5,i}[B(b_1 - b_2)^2] + J_{6,i}[V(v_1 - v_2)^2] + J_{7,i}[A.B(a_1 b_1 - a_2 b_2)^2] \quad \text{Eq. (9)}$$

where subscripts 1 and 2 denote the cosolvent and solvent, respectively, E is the excess molar refraction, S is the dipolarity/polarizability of the solute, A and B denotes the solute's hydrogen-bond acidity and basicity, and V is the McGowan characteristic volume of the solute in units of $(cm^3 . mol^{-1})/100$.

Table 2. Regression results of the CNIBS/R-K equation model.

T(K)	288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15	328.15
Ethanol + Hexane									
J_0	4.495	4.552	4.332	4.233	4.199	4.278	4.122	4.113	4.042
J_1	-3.996	-3.823	-3.589	-3.323	-3.584	-3.607	-3.549	-3.586	-3.528
J_2	4.702	4.689	4.408	4.015	3.857	3.801	3.664	3.641	3.584
100RD	2.8	1.2	1.4	0.7	0.8	0.6	0.9	0.4	1.0
Isopropyl alcohol + Hexane									
J_0	4.655	4.608	4.380	4.273	4.274	4.223	4.111	4.084	-
J_1	-5.305	-5.119	-4.861	-4.809	-4.935	-4.996	-4.906	-4.921	-
J_2	5.417	5.125	4.809	4.679	4.737	4.581	4.412	4.313	-
100RD	0.7	0.8	1.1	0.9	0.7	0.3	0.6	0.8	-
Chloroform + Hexane									
J_0	3.548	3.547	3.203	3.178	3.268	3.311	3.248	3.284	-
J_1	-3.269	-2.954	-3.071	-3.045	-3.000	-3.105	-3.092	-3.121	-
J_2	3.164	3.009	2.819	2.957	2.797	2.703	2.587	2.482	-
100RD	1.1	0.8	1.6	1.4	1.3	0.9	0.9	1.2	-
Acetone + Hexane									
J_0	3.606	3.482	3.312	3.351	3.514	3.659	3.468	-	-
J_1	-3.796	-3.739	-3.674	-3.776	-3.930	-4.188	-4.173	-	-
J_2	4.269	4.595	4.488	4.568	4.569	4.623	4.728	-	-
100RD	1.4	0.5	0.4	1.4	1.9	3.5	3.3	-	-
Acetone + Water									
J_0	11.985	11.748	11.446	11.082	10.726	10.775	10.638	-	-
J_1	-7.458	-9.266	-10.236	-9.934	-11.130	-10.352	-9.743	-	-
J_2	15.348	12.294	10.140	10.142	8.932	10.124	11.923	-	-
100RD	5.7	3.6	4.3	2.7	2.3	1.3	2.3	-	-

Table 3. Regression results of the modified Wilson model.

T(K)	288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15	328.15
Ethanol + Hexane									
Λ_{12}	0.175	0.535	0.755	1.208	1.019	1.620	2.159	3.714	8.845
Λ_{21}	5.711	5.103	5.048	4.846	5.692	6.09	6.860	7.941	10.034
100RD	5.4	5.1	5.0	4.3	3.3	3.1	2.5	2.1	1.2
Isopropyl alcohol + Hexane									
Λ_{12}	0.152	0.132	0.122	0.113	0.098	-0.002	-4.2×10^{-8}	-5.315	-
Λ_{21}	6.595	7.569	8.204	8.882	10.186	12.423	7.227	8.331	-
100RD	6.4	4.3	3.4	3.0	3.4	3.7	12.97	22.6	-
Chloroform + Hexane									
Λ_{12}	0.211	0.187	0.199	0.180	0.163	0.154	0.188	0.354	-
Λ_{21}	4.740	5.338	5.030	5.567	6.120	6.474	6.738	6.511	-
100RD	3.4	1.9	2.8	2.5	1.4	1.4	1.2	0.9	-
Acetone + Hexane									
Λ_{12}	0.253	0.231	0.216	0.186	0.157	0.130	0.118	-	-
Λ_{21}	3.955	4.324	4.633	5.367	6.383	7.721	8.489	-	-
100RD	8.3	7.6	7.2	6.0	4.8	4.3	4.3	-	-
Acetone + Water									
Λ_{12}	5.307	405.970	5.0×10^{7}	1.5×10^{7}	1.5×10^{7}	2.479×10^{7}	4.1×10^{7}	-	-
Λ_{21}	7.008	7.199	7.789	8.145	8.561	9.188	9.9	-	-
100RD	8.7	10.4	12.58	12.6	15.2	17.2	18.2	-	-

Table 4. Regression results of the GSM.

T(K)	288.15	293.15	298.15	303.15	308.15	313.15	318.15	323.15	328.15
Ethanol + Hexane									
B_0	-5.216	-4.886	-4.532	-4.278	-4.072	-3.902	-3.629	-3.448	-3.211
B_1	11.667	11.335	10.602	10.086	10.219	10.226	9.824	9.761	9.449
B_2	-15.335	-14.991	-14.114	-13.319	-14.104	-14.267	-13.957	-14.091	-13.817
B_3	7.136	6.867	6.439	5.981	6.531	6.586	6.488	6.584	6.448
B_4	-	-	-	-	-	-	-	-	-
100RD	10.4	10.1	9.53	8.3	8.0	7.8	7.6	7.6	7.3
Isopropyl alcohol + Hexane									
B_0	-5.182	-4.852	-4.500	-4.241	-4.034	-3.868	-3.595	-3.414	-
B_1	13.283	12.806	12.060	11.760	11.789	11.755	11.359	11.233	-
B_2	-19.821	-19.261	-18.270	-18.030	-18.435	-18.622	-18.227	-18.230	-
B_3	10.020	9.684	9.183	9.092	9.360	9.520	9.333	9.353	-
B_4	-	-	-	-	-	-	-	-	-
100RD	12.0	11.2	10.3	10.4	10.5	10.4	9.9	9.9	-

Table 4. *(Continued)*

Chloroform + Hexane									
B_0	-5.223	-4.893	-4.534	-4.271	-4.066	-3.900	-3.628	-3.446	-
B_1	9.636	9.121	8.716	8.543	8.509	8.654	8.434	8.426	-
B_2	-12.903	-12.026	-11.945	-11.859	-11.809	-12.260	-12.152	-12.265	-
B_3	6.188	5.607	5.785	5.742	5.649	5.924	5.895	5.952	-
B_4	-	-	-	-	-	-	-	-	-
100RD	6.7	6.4	6.0	6.3	5.9	5.7	5.5	5.3	-
Acetone + Hexane									
B_0	-5.221	-4.872	-4.515	-4.244	-4.034	-3.851	-3.576	-	-
B_1	10.849	10.382	9.882	9.795	9.981	10.217	9.80	-	-
B_2	-14.585	-14.132	-13.741	-13.956	-14.516	-15.256	-15.034	-	-
B_3	7.234	7.008	6.863	6.981	7.242	7.641	7.617	-	-
B_4	-	-	-	-	-	-	-	-	-
100RD	9.8	10.2	9.7	9.6	9.7	10.1	10.2	-	-
Acetone + Water									
B_0	-8.244	-8.29	-7.611	-7.317	-7.187	-6.993	-6.833	-	-
B_1	33.875	34.001	33.047	32.222	32.770	32.503	32.651	-	-
B_2	-60.807	-61.448	-59.834	-58.685	-60.580	-60.477	-61.645	-	-
B_3	33.344	33.751	32.779	32.252	33.841	33.625	34.588	-	-
B_4	-	-	-	-	-	-	-	-	-
100RD	11.2	9.2	8.3	7.0	6.8	7.7	9.2	-	-

Table 5. Regression results of the Jouyban-Acree model and Jouyban-Acree-van't Hoff model.

Parameters			
Jouyban-Acree		**Jouyban-Acree-van't Hoff**	
Ethanol + Hexane			
J_0	1310.974	A_1	3.361
J_1	-1113.135	A_2	10.963
J_2	1245.775	B_1	-1510.962
		B_2	-4662.335
		J_0	1311.086
		J_1	-1107.479
		J_2	1249.109
100RD	1.6	*100RD*	1.8
Isopropyl alcohol + Hexane			
J_0	1320.716	A_1	4.094
J_1	-1519.304	A_2	10.972
J_2	1452.264	B_1	-1705.927
		B_2	-4664.149
		J_0	1320.969
		J_1	-1512.459
		J_2	1456.048
100RD	1.4	*100RD*	1.8
Chloroform + Hexane			
J_0	1013.883	A_1	6.724
J_1	-939.524	A_2	11.321
J_2	860.200	B_1	-2622.749
		B_2	-4769.569
		J_0	1012.242
		J_1	-928.611
		J_2	858.227
100RD	2.0	*100RD*	2.0
Acetone + Hexane			
J_0	1053.956	A_1	4.398
J_1	-1177.063	A_2	12.884
J_2	1374.822	B_1	-1798.698
		B_2	-5239.721
		J_0	1053.218
		J_1	-1165.082
		J_2	1376.022
100RD	2.9	*100RD*	2.6
Acetone + Water			
J_0	3392.677	A_1	4.509
J_1	-2936.341	A_2	8.484
J_2	3421.345	B_1	-1830.508
		B_2	-4863.673
		J_0	3380.286
		J_1	-2968.552
		J_2	3316.102
100RD	4.2	*100RD*	5.6

The *c*, *e*, *s*, *a*, *b* and *v* (solvent's coefficients), which depend upon the solvent under investigation. The *e* is the tendency of the phase to interact with solutes through polarizability-type interactions, *s* is a measure of the solvent phase dipolarity/polarity, the *a*- and *b*-coefficients represent the solvent phase hydrogen-bond basicity and acidity, respectively and *v* is the general dispersion interaction energy between the solute and solvent phase. Numerical values of the coefficients for water-to-organic solvent systems have been reported in the literature [17] and tabulated in Table 6.

Table 6. The Abraham parameters of the investigated solvents taken from a reference.[17]

Solvent	*c*	*e*	*s*	*a*	*b*	*v*
2-Propanol	0.099	0.343	–1.049	0.406	–3.827	4.033
Ethanol	0.222	0.471	–1.035	0.326	–3.596	3.857
Acetone	0.313	0.312	-0.121	-0.608	-4.753	3.942
Hexane	0.333	0.560	-1.710	-3.578	-4.939	4.463
Chloroform	0.191	0.105	-0.403	-3.112	-3.514	4.395
Water	-0.994	0.577	2.549	3.813	4.481	-3.869

By simplifying of Eq. 9 for a given drug/drug like compound, the Jouyban-Acree-van't Hoff model combined with the Abraham parameters of solvent coefficients for calculating the solubility in mixed solvents at various temperatures is expressed as Eq. 10. The *J* terms are the model constants computed using a no intercept least square analysis.

$$\ln x_{m,T} = w_1(A_1 + \frac{B_1}{T}) + w_2(A_2 + \frac{B_2}{T}) + (\frac{w_1 w_2}{T})\left\{\begin{array}{l} J_1 + J_2(c_1 - c_2)^2 + J_3(e_1 - e_2)^2 + J_4(s_1 - s_2)^2 + J_5(a_1 - a_2)^2 + J_6(b_1 - b_2)^2 \\ + J_7(v_1 - v_2)^2 + J_8(a_1 - a_2)^2(b_1 - b_2)^2 \end{array}\right\} + (\frac{w_1 w_2 (w_1 - w_2)}{T})\left\{\begin{array}{l} J_9 + J_{10}(c_1 - c_2)^2 + J_{11}(e_1 - e_2)^2 + J_{12}(s_1 - s_2)^2 + J_{13}(a_1 - a_2)^2 \\ + J_{14}(b_1 - b_2)^2 + J_{15}(v_1 - v_2)^2 + J_{16}(a_1 - a_2)^2(b_1 - b_2)^2 \end{array}\right\} + (\frac{w_1 w_2 (w_1 - w_2)^2}{T})\left\{\begin{array}{l} J_{17} + J_{18}(c_1 - c_2)^2 + J_{19}(e_1 - e_2)^2 + J_{20}(s_1 - s_2)^2 + J_{21}(a_1 - a_2)^2 \\ + J_{22}(b_1 - b_2)^2 + J_{23}(v_1 - v_2)^2 + J_{24}(a_1 - a_2)^2(b_1 - b_2)^2 \end{array}\right\} \quad \text{Eq. (10)}$$

$$\ln x_{m,T} = w_1(4.183 - \frac{1766.916}{T}) + w_2(11.783 - \frac{5095.935}{T}) + (\frac{w_1 w_2}{T})\left\{1265.197 + 27.334\ (a_1 - a_2)^2\right\} + (\frac{w_1 w_2 (w_1 - w_2)}{T})\left\{\begin{array}{l} -2524.032\ (c_1 - c_2)^2 - 8081.901\ (e_1 - e_2)^2 \\ -100.578\ (a_1 - a_2)^2 \end{array}\right\} + (\frac{w_1 w_2 (w_1 - w_2)^2}{T})\left\{\begin{array}{l} 405.686\ (s_1 - s_2)^2 + 134.302\ (a_1 - a_2)^2 \\ -9.898\ (a_1 - a_2)^2(b_1 - b_2)^2 \end{array}\right\} \quad \text{Eq. (11)}$$

All obtained solubility data of benzoic acid in the binary solvent mixtures at various temperatures were fitted to Eq. 10 and the trained version of Jouyban-Acree-van't Hoff model combined with the Abraham parameters of solvent coefficients, as a QSPR model, after excluding nonsignificant model constant (p>0.05) is Eq.11.

The back-calculated *MRDs%* are 8.5% for solubility of benzoic acid in {ethanol (1) + hexane (2)} mixture, 10.7% in {isopropyl alcohol (1) + hexane (2)} mixture, 13.6% in {chloroform (1) + hexane (2)} mixture, 11.8% in {acetone (1) + hexane (2)} mixture and 157.7% in {acetone (1) + water (2)} mixture. The overall predicted *MRD%* is 35.2 %.

Conclusion

In addition to reanalyzing of mathematical computations published by Sandeepa *et al.*, some further computational methods are also provided in this short communication to be employed in the future research works. Furthermore, discussions regarding the Jouyban–Acree–van't Hoff model and its combined version with the Abraham solvation parameters are also given here. This combined model provide a generally trained model to predict the solubility of benzoic acid in a given cosolvent + water mixtures.

Conflict of interests

The authors claim that there is no conflict of interest.

References

1. Sandeepa K, Ravi Kumar K, Neeharika TS, Satyavathi B, Thella PK. Solubility measurement and thermodynamic modeling of benzoic acid in monosolvents and binary mixtures. J Chem Eng Data. 2018;63(6):2028-37. doi:10.1021/acs.jced.8b00025
2. Furia TE. CRC Handbook of Food Additives. Second ed. Boca Raton, FL: CRC Press; 1981.
3. Lillard B. Practical druggist and pharmaceutical review of reviews. Lillard & Company; 1904.
4. Wilson CO, Gisvold Ole, Block JH. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical. Lippincott Williams & Wilkins; 2004. p. 234.
5. Jouyban A, Fakhree MAA, Shayanfar A. Solubility prediction methods for drug/drug like molecules. Recent Pat Chem Eng. 2010;1(3):220-31. doi:10.2174/22113347108010302 20
6. http://www.spss.com.hk/software/statistics/.
7. Barzegar-Jalali M, Jouyban-Gharamaleki A. A general model from theoretical cosolvency models. Int J Pharm. 1997;152(2):247-50. doi:10.1016/S0378-5173(97)04922-3
8. Jouyban-Gharamaleki A. The modified Wilson model and predicting drug solubility in water-cosolvent mixtures. Chem Pharm Bull. 1998;46(6):1058-61. doi:10.1248/cpb.46.1058
9. Acree Jr WE. Mathematical representation of thermodynamic properties: Part 2. Derivation of the combined nearly ideal binary solvent (NIBS)/Redlich-Kister mathematical representation from a two-body and three-body interactional mixing model. Thermochim Acta. 1992;198(1):71-9. doi:10.1016/0040-6031(92)85059-5
10. Jouyban A, Acree Jr WE. Mathematical derivation of the Jouyban-Acree model to represent solute solubility data in mixed solvents at various temperatures. J Mol Liq. 2018;256:541-7. doi:10.1016/j.molliq.2018.01.171
11. Ruidaz Martinez MA, Rodriguez SJ, Neita PC, Cristancho DM, Martinez F. Performance of the Jouyban-Acree model for correlating the solubility of indomethacin and ethylhexyl triazone in ethyl acetate+ ethanol mixtures. Vitae. 2010;17(3):309-16.
12. Patel SV, Patel S. Prediction of the solubility in lipidic solvent mixture: investigation of the modeling approach and thermodynamic analysis of solubility. Eur J Pharm Sci. 2015;77:161-9. doi:10.1016/j.ejps.2015.06.014
13. Jouyban A, Fakhree MAA, Acree Jr WE. Comment on "Measurement and correlation of solubilities of (Z)-2-(2-aminothiazol-4-Yl)-2-methoxyiminoacetic acid in different pure solvents and binary mixtures of water+(ethanol, methanol, or glycol)". J Chem Eng Data. 2012;57(4):1344-6. doi:10.1021/je201340e
14. Sardari F, Jouyban A. Solubility of nifedipine in ethanol+ water and propylene glycol+ water mixtures at 293.2 to 313.2 K. Ind Eng Chem Res. 2013;52(40):14353-8. doi:10.1021/ie402588t
15. Jouyban A, Acree Jr WE. Solubility prediction in non-aqueous binary solvents using a combination of Jouyban-Acree and Abraham models. Fluid Phase Equilib. 2006;249(1-2):24-32. doi:10.1016/j.fluid.2006.08.016
16. Jouyban A, Soltanpour S, Soltani S, Chan H, Acree Jr WE. Solubility prediction of drugs in water-cosolvent mixtures using Abraham solvation parameters. J Pharm Pharm Sci. 2007;10(3):263-77.
17. Acree Jr WE, Ramirez AM, Cheeran S, Martinez F. Determination of Abraham model solute descriptors and preferential solvation from measured solubilities for 4-nitropyrazole dissolved in binary aqueous-organic solvent mixtures. Phys Chem Liq. 2017;55(5):605-16. doi:10.1080/00319104.2016.1250272