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Review

Solubility and solution thermodynamics of novel pyrazolo chalcone derivatives in various solvents from 298.15 K to 328.15 K

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ABSTRACT

Some novel pyrazolo chalcone derivatives have been synthesized and characterization of these synthesized compounds was done by IR, ^{1}H NMR, ^{13}C NMR and mass analysis. The solubility of pyrazolo chalcone derivatives in methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, ethyl acetate and acetonitrile was measured by gravimetric method over a temperature range (298.15 to 328.15) K at atmospheric pressure. The solubility of synthesized compounds is found to increase linearly with temperature. Further, in alcoholic solvents, solubility is maximum in 1-pentanol and minimum in methanol whereas in non-alcoholic solvents, solubility is greater in ethyl acetate and minimum in acetonitrile. The experimental solubility data were correlated with temperature by modified Apelblat and Buchowski-Ksiazczak λ*h* equations. The experimental data and model parameters would be useful for optimizing the process of purification. Some thermodynamic parameters such as dissolution enthalpy, Gibb's free energy and entropy of mixing have also been calculated by Van't Hoff analysis. Further, excess enthalpy of solutions has been calculated using Buchowski-Ksiazczak λ*h* equation.

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1. Introduction

Chalcones, considered to be the precursor of flavonoids and isoflavonoids are abundant in edible plants as well as useful for the synthesis of several derivatives like cyanopyridines [1], pyrazolines isoxazoles [2] and pyrimidines [3]. These chalcones containing keto ethylenic group demonstrate various biological activities such as anti-inflammatory [4], antiherbicidal [5], anti-HIV [6], anti-ulcer [7] and anti-cancer [8] etc. Due to these biological applications, it was of our interest to study the behaviour of these pyrazolo chalcones in solutions which may be useful for their further applications in different fields.

The ability of a chemical compound to elicit a pharmacological/therapeutic effect is related to its various physicochemical properties. Solubility is one of the properties which provide preliminary information on the nature of the tested compound. Solubility behaviour of a compound is an important factor affecting their bioavailability [9]. Further, solubility data provides useful information to understanding of intermolecular

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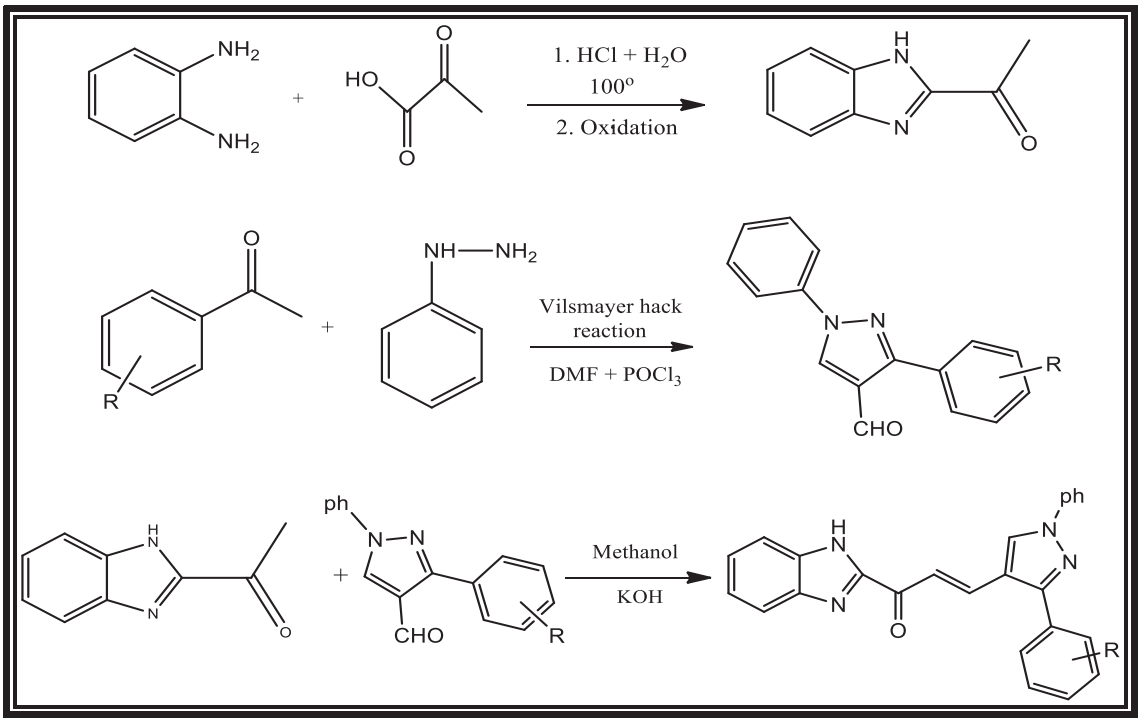

Fig. 1. Reaction Scheme for synthesized pyrazolo chalcone derivatives.

forces-solution and structure property relationship [10]. By using this data one can design process pharmaceutical dosage form and drug discovery process [11,12]. It is also important for synthesis and evaluation of the separation process [13,14]. Study of temperature dependence solubility data provides the explanation of molecular mechanisms involved in the respective drug dissolution process [15]. The data has been useful in drug design, formulation, production, distillation and crystallization based on separation [16] etc. Solubility data may be useful to understand various biological processes [17,18].

Because of the continuing interest and marvellous biological activity of chalcone derivatives, the solubility of synthesized compounds has been studied in different solvents and temperatures. These data were correlated with a modified Apelblat and Buchowski-Ksiazczak λ*h* models. Further, using solubility data, some thermodynamic parameters such as dissolution enthalpy, Gibb's free energy and entropy of mixing were also evaluated.

2. Experimental

The chemicals used in the synthesis of different chalcone compounds are *o*-phenyledine diamine, glacial acetic acid, phenyl hydrazine and different substituted acetophenones etc. These chemicals were purchased from Spectochem Pvt. Ltd. (Mumbai, India) as well as LOBA Chemie Pvt. Ltd. and the mole fraction purities of these chemicals were of 98.5–99.5%. The solvents used in solubility determination were of Analytical Reagent (AR) grade and were further purified according to reported method [19]. All the distilled solvents were stored over dry molecular sieves. The purity of solvents was checked by GC–MS (SHIMADZU Model-QP- 2010).

2.1. Synthesis

A methanolic solution of different 1-(1H-benzo[*d*]imidazole-2-yl) ethan-1-one (0.01 mol), pyrazolo aldehyde (0.008–0.007 mol) and potassium hydroxide (0.04 mol) was stirred at room temperature for 1 h. The completion of reaction was confirmed by analytical thin layer chromatography (TLC) (Performed on aluminium coated plates Gel 60F254 (E. Merck)) using (0.6:0.4-Hexane: Ethyl acetate) as mobile phase. After completion of reaction, the reaction mass was poured in to crushed ice and the resultant solid was filtered, washed with methanol to remove unreacted reagents and dried under vacuum to give crude product.

The reaction scheme is given in Fig. 1.

Table 1
Physical properties of synthesized chalcone derivatives.

Compound	-R	Molecular formula	Average molar mass	Yield (%)	R_f^a value	T_{fus}/K	Electro-negativity
AH-1	3-methoxy	$C_{26}H_{20}N_4O_2$	420.158	80	0.84	504.28	2.26
AH-2	-H	$C_{25}H_{18}N_4O$	390.446	80	0.84	543.65	–
AH-3	4-chloro	$C_{25}H_{17}ClN_4O$	424.880	80	0.80	540.90	3.00
AH-4	3, 4-dimethoxy	$C_{27}H_{22}N_4O_3$	450.169	81	0.71	524.11	2.25
AH-5	4-flouro	$C_{25}H_{17}FN_4O$	408.440	85	0.88	555.43	4.00
AH-6	2-chloro	$C_{25}H_{17}ClN_4O$	424.110	86	0.80	554.67	2.97
AH-7	4-methoxy	$C_{26}H_{20}N_4O_2$	420.158	89	0.88	535.64	2.24
AH-8	3-nitro	$C_{25}H_{17}N_5O_3$	436.136	83	0.83	523.01	≈2.8

R_f^a - Retention factor.
T_{fus} - Melting point.
[a] 0.6:0.4-Hexane: Ethyl acetate.

Table 2
Experimental mole fraction solubilities (x_i) and relative deviation (RD) of chalcone derivatives in selected solvents at different temperatures at experimental pressure p = 0.1 MPa.

$T(K)$	$x_i \cdot 10^3$	$x_{ci}{}^a \cdot 10^3$	$100 \cdot RD^a$	$x_{ci}{}^b \cdot 10^3$	$100 \cdot RD^b$	$x_i \cdot 10^3$	$x_{ci}{}^a \cdot 10^3$	$100 \cdot RD^a$	$x_{ci}{}^b \cdot 10^3$	$100 \cdot RD^b$
Methanol										
AH-1						AH-2				
298.15	0.0271	0.0272	−0.4431	0.0275	−1.5509	0.0554	0.0561	−1.1905	0.0580	−4.7979
303.15	0.0315	0.0315	0.1268	0.0315	0.1268	0.0653	0.0669	−2.4502	0.0668	−2.4502
308.15	0.0363	0.0361	0.5235	0.0359	1.0747	0.0808	0.0783	3.0461	0.0765	5.1511
313.15	0.0412	0.0411	0.3153	0.0408	1.0429	0.0883	0.0899	−1.8120	0.0873	1.0193
318.15	0.0462	0.0464	−0.3894	0.0462	0.0433	0.0987	0.1013	−2.6551	0.0992	−0.6283
323.15	0.0515	0.0519	−0.7767	0.0520	−0.9709	0.1153	0.1121	2.7754	0.1122	2.5152
328.15	0.0581	0.0577	0.6029	0.0584	−0.6029	0.1229	0.1221	0.6348	0.1265	−3.1087
AH-3						AH-4				
298.15	0.0406	0.0429	−5.6650	0.0461	0.7322	0.0304	0.0307	−0.9536	0.0312	−2.5978
303.15	0.0510	0.0557	−9.2157	0.0553	1.5929	0.0360	0.0355	1.4163	0.0355	1.4162
308.15	0.0674	0.0696	−3.2947	0.0659	−1.7839	0.0406	0.0406	0.0984	0.0403	1.0827
313.15	0.0790	0.0840	6.3291	0.0781	−0.9056	0.0447	0.0459	−2.7305	0.0455	−1.6115
318.15	0.0936	0.0979	−4.5493	0.0921	1.5841	0.0502	0.0515	−2.6305	0.0512	−1.8334
323.15	0.1050	0.0111	−5.7140	0.1080	−2.5161	0.0550	0.0572	−4.0000	0.0574	−4.0000
328.15	0.1167	0.1214	−4.0185	0.1260	−0.0696	0.0653	0.0631	3.3394	0.0574	2.1140
AH-5						AH-6				
298.15	0.5601	0.5595	0.1125	0.5596	0.1125	0.0904	0.0929	−2.7768	0.0967	−6.9808
303.15	0.5690	0.5698	−0.1406	0.5698	−0.1406	0.1160	0.1118	3.6207	0.1116	3.7931
308.15	0.5779	0.5799	−0.3548	0.5798	−0.3375	0.1332	0.1315	1.2392	0.1283	3.6425
313.15	0.5880	0.5898	−0.3061	0.5897	−0.2891	0.1490	0.1514	−1.6107	0.1467	1.4765
318.15	0.5964	0.5995	−0.5198	0.5995	−0.5030	0.1679	0.1709	−1.8049	0.1672	0.3991
323.15	0.6060	0.6091	−0.5115	0.6091	−0.4950	0.1870	0.1894	−1.2834	0.1897	−1.4438
328.15	0.6189	0.6185	0.0662	0.6186	0.0662	0.2092	0.2061	1.4865	0.2144	−2.4807
AH-7						AH-8				
298.15	0.1454	0.1449	0.3576	0.1449	0.3576	0.0404	0.0409	−1.3129	0.0419	−3.7899
303.15	0.1488	0.1503	−1.0081	0.1503	−1.0081	0.0485	0.0475	2.0619	0.0475	2.0619
308.15	0.1547	0.1556	−0.6078	0.1556	−0.6078	0.0550	0.0544	1.1269	0.0535	2.7626
313.15	0.1600	0.1609	−0.5625	0.1610	−0.5625	0.0590	0.0613	−3.8983	0.0601	−1.8644
318.15	0.1665	0.1663	0.1261	0.1663	0.1261	0.0659	0.0682	−3.4901	0.0673	−2.1244
323.15	0.1700	0.1717	−1.0000	0.1717	−1.0000	0.0740	0.0749	−1.2162	0.0750	−1.3514
328.15	0.1767	0.1771	−0.2037	0.1771	−0.1471	0.0821	0.0812	1.0962	0.0833	−1.5834
Ethanol										
AH-1						AH-2				
298.15	0.0724	0.0728	−0.7131	0.0763	−5.4450	0.0848	0.0842	−1.1905	0.0763	−4.7980
303.15	0.0850	0.0886	−4.2753	0.0883	−3.8824	0.0940	0.0958	−2.4502	0.0883	−2.4502
308.15	0.1056	0.1050	0.5097	0.1017	3.6476	0.1064	0.1081	3.0461	0.1018	5.1511
313.15	0.1213	0.1214	−0.0726	0.1167	3.7923	0.1230	0.1208	−1.8120	0.1167	1.0193
318.15	0.1361	0.1371	−0.7296	0.1333	2.0645	0.1348	0.1339	−2.6551	0.1333	−0.6283
323.15	0.1482	0.1515	−2.2141	0.1516	−2.2735	0.1460	0.1472	2.7754	0.1516	2.5152
328.15	0.1651	0.1640	0.6174	0.1717	−4.0291	0.1601	0.1606	0.6348	0.1718	−3.1087
AH-3						AH-4				
298.15	0.1017	0.1011	0.6339	0.1011	0.7322	0.0391	0.0389	0.6958	0.0402	10.0130
303.15	0.1130	0.1113	1.5044	0.1113	1.5929	0.0500	0.0487	−1.9149	0.0486	6.0638
308.15	0.1199	0.1223	−1.9506	0.1223	−1.7839	0.0588	0.0596	−1.5214	0.0584	4.3952
313.15	0.1325	0.1339	−1.0566	0.1339	−0.9057	0.0716	0.7160	1.7886	0.0697	5.1220
318.15	0.1484	0.1461	1.5167	0.1461	1.5841	0.0846	0.0844	0.7266	0.0828	1.1714
323.15	0.1550	0.1591	−2.6451	0.1591	−2.5161	0.1000	0.0977	−0.8219	0.0978	−3.8356
328.15	0.1725	0.1728	−0.1855	0.1728	−0.0696	0.1111	0.1112	−0.2935	0.1149	−7.2254
AH-5						AH-6				
298.15	0.8143	0.8146	−0.0343	0.8151	−0.1081	0.1051	0.1353	−28.7350	0.1094	−3.9961
303.15	0.8280	0.2820	0.3623	0.8284	−0.0483	0.1253	0.1562	−24.6610	0.1242	0.9577
308.15	0.8393	0.8416	−0.2717	0.8414	−0.2478	0.1451	0.1774	−22.2940	0.1404	3.2814
313.15	0.8550	0.8547	0.0350	0.8542	0.0936	0.1567	0.1983	−26.5480	0.1580	−0.7658
318.15	0.8689	0.8675	0.1588	0.8667	0.2509	0.1786	0.2183	−22.2010	0.1773	0.8061
323.15	0.8790	0.8801	−0.1251	0.8791	−0.0114	0.1950	0.2372	−21.6410	0.1982	−1.5897
328.15	0.8930	0.8925	0.0593	0.8912	0.1937	0.2172	0.2542	−17.0240	0.2208	−1.6481
AH-7						AH-8				
298.15	0.3519	0.3539	−0.5626	0.3539	−0.5626	0.0553	0.0553	0.0000	0.0547	1.0850
303.15	0.3720	0.3697	0.6183	0.3697	0.6183	0.0620	0.0629	−1.4516	0.0630	−1.4516
308.15	0.3855	0.3858	−0.0752	0.3857	−0.0493	0.0701	0.0716	−2.2127	0.0721	−2.9265
313.15	0.3986	0.4019	−0.8254	0.4019	−0.8254	0.0842	0.0816	3.0879	0.0823	2.2565
318.15	0.4195	0.4182	0.3051	0.4182	0.3051	0.0946	0.0929	1.8074	0.0935	1.1732
323.15	0.4300	0.4346	−1.0674	0.4346	−1.0674	0.1032	0.1058	−2.5194	0.1058	−2.5194
328.15	0.4518	0.4512	0.1416	0.4512	0.1416	0.1194	0.1205	−0.8875	0.1193	0.2009
1-propanol										
AH-1						AH-2				
298.15	0.1256	0.1257	−0.0876	0.1291	−2.7948	0.1352	0.1353	−0.1110	0.1392	−2.9967
303.15	0.1453	0.1453	0.0138	0.1454	−0.0551	0.1523	0.1562	−2.5607	0.1560	−2.4294
308.15	0.1657	0.1655	0.0906	0.1632	1.4790	0.1785	0.1774	0.6385	0.1742	2.4308
313.15	0.1865	0.1858	0.3753	0.1824	2.1984	0.1890	0.1983	−4.9206	0.1938	−2.5397
318.15	0.2063	0.2058	0.2569	0.2032	1.5169	0.2154	0.2184	−1.4116	0.2149	0.2600
323.15	0.2310	0.2250	2.5974	0.2256	2.3377	0.2260	0.2372	−4.9558	0.2375	−5.0443

Table 2 (*continued*)

$T(K)$	$x_i \cdot 10^3$	$x_{ci}^a \cdot 10^3$	$100 \cdot RD^a$	$x_{ci}^b \cdot 10^3$	$100 \cdot RD^b$	$x_i \cdot 10^3$	$x_{ci}^a \cdot 10^3$	$100 \cdot RD^a$	$x_{ci}^b \cdot 10^3$	$100 \cdot RD^b$
328.15	0.2449	0.2432	0.6739	0.2497	−1.9808	0.2551	0.2541	0.3842	0.2617	−2.5561
AH-3						AH-4				
298.15	0.0835	0.0840	−0.5627	0.0972	−2.7948	0.1251	0.1255	−0.2877	0.1254	0.0000
303.15	0.1030	0.1023	0.6796	0.1080	−0.0551	0.1400	0.1386	1.0000	0.1386	0.0000
308.15	0.1213	0.1202	0.9232	0.1195	1.4790	0.1503	0.1527	−1.5901	0.1526	0.0000
313.15	0.1322	0.1364	−3.1770	0.1318	2.1984	0.1670	0.1676	−0.3593	0.1676	0.0000
318.15	0.1501	0.1499	0.1599	0.1449	1.5170	0.1854	0.1836	0.9922	0.1835	0.0000
323.15	0.1580	0.1599	−1.2025	0.1589	2.3377	0.2000	0.2004	−0.2000	0.2003	0.0000
328.15	0.1673	0.1657	0.9623	0.1738	−1.9808	0.2200	0.2182	0.8272	0.2181	0.0000
AH-5						AH-6				
298.15	1.0377	1.0340	0.3585	1.0341	0.1754	0.1568	0.1566	13.6890	0.1548	1.2503
303.15	1.0560	1.0562	−0.0189	1.0562	−0.0852	0.1670	0.1675	6.4671	0.1676	−0.2994
308.15	1.0733	1.0782	−0.4528	1.0781	−0.4062	0.1769	0.1796	−0.3110	0.1809	−2.2335
313.15	1.0930	1.0782	1.3541	1.0997	−0.4666	0.1890	0.1931	−4.9206	0.1948	−3.0688
318.15	1.1153	1.1212	−0.5317	1.1211	−0.2717	0.2053	0.2080	−6.3602	0.2093	−1.8798
323.15	1.1450	1.1422	0.2445	1.1422	0.5852	0.2200	0.2245	−7.8182	0.2244	−1.9546
328.15	1.1679	1.1630	0.4204	1.1630	0.8571	0.2440	0.2428	−4.1633	0.2401	1.6964
AH-7						AH-8				
298.15	0.4901	0.4934	−0.6651	0.4939	−0.7671	0.1145	0.1152	−0.5762	0.1196	−4.4177
303.15	0.5200	0.5160	0.7692	0.5165	0.6731	0.1350	0.1376	−1.9259	0.1374	−1.7037
308.15	0.5407	0.5388	0.3588	0.5394	0.2478	0.1641	0.1609	1.9261	0.1571	4.2424
313.15	0.5650	0.5619	0.5487	0.5625	0.4425	0.1753	0.1843	−5.1341	0.1789	−1.9966
318.15	0.5856	0.5853	0.0512	0.5858	−0.0512	0.2057	0.2071	−0.6953	0.2028	1.4441
323.15	0.6150	0.6088	1.0081	0.6093	0.9106	0.2256	0.2287	−1.3741	0.2291	−1.4628
328.15	0.6278	0.6325	−0.7567	0.6331	−0.8523	0.2505	0.2483	0.8901	0.2578	−2.8619
1-butanol										
AH-1						AH-2				
298.15	0.1701	0.1684	0.9819	0.1687	0.8056	0.2477	0.2465	0.4764	0.2535	2.3740
303.15	0.1854	0.1882	−1.4993	0.1885	−1.6611	0.2750	0.2717	1.2000	0.2750	1.2000
308.15	0.2115	0.2096	0.9171	0.2099	0.7753	0.2988	0.3008	−0.6727	0.3040	−1.8106
313.15	0.2299	0.2326	−1.1744	0.2330	−1.3484	0.335	0.3345	0.1493	0.3540	−1.3134
318.15	0.2584	0.2573	0.4257	0.2577	0.2709	0.3742	0.3735	0.1924	0.3875	−0.8231
323.15	0.2853	0.2838	0.5258	0.2842	0.3856	0.4250	0.4186	1.5059	0.4235	1.6235
328.15	0.3115	0.3121	−0.1830	0.3125	−0.3114	0.4653	0.4708	−1.1886	0.4618	0.7458
AH-3						AH-4				
298.15	0.1502	0.1507	−0.3529	0.1553	−3.4161	0.1596	0.1633	−2.3119	0.1730	−8.3892
303.15	0.1750	0.1754	−0.2286	0.1752	−0.0571	0.2090	0.2025	3.1100	0.2020	3.3971
308.15	0.2013	0.2005	0.4073	0.1967	2.2949	0.2445	0.2433	0.4745	0.2345	4.1152
313.15	0.2156	0.2255	−4.5918	0.2201	−2.0872	0.2800	0.2839	−1.3929	0.2711	3.2500
318.15	0.2398	0.2797	−16.649	0.2455	−2.3438	0.3206	0.3222	−0.5022	0.3119	2.7418
323.15	0.2580	0.2724	−5.5814	0.2728	−5.7364	0.3500	0.3564	−1.8286	0.3573	−2.0571
328.15	0.2952	0.2931	0.7181	0.3022	−2.3643	0.3899	0.3846	1.3770	0.4076	−4.4696
AH-5						AH-6				
298.15	1.5823	1.5846	−0.1460	1.5848	−0.1650	0.2942	0.2960	−0.6221	0.2960	−0.6221
303.15	1.6000	1.6008	−0.0500	1.6009	−0.0563	0.3300	0.3296	0.1212	0.3296	0.1212
308.15	1.6161	1.6167	−0.0396	1.6166	−0.0396	0.3543	0.3657	−3.2264	0.3657	−3.2546
313.15	1.6480	1.6321	0.9648	1.6320	0.9648	0.4000	0.4045	−1.1250	0.4044	−1.1250
318.15	1.6484	1.6471	0.0758	1.6471	0.0758	0.4446	0.4459	−0.2879	0.4459	−0.2879
323.15	1.6530	1.6618	−0.5324	1.6618	−0.5384	0.5000	0.4901	1.9800	0.4900	2.0000
328.15	1.6743	1.6760	−0.1033	1.6762	−0.1213	0.5333	0.5371	−0.7125	0.5371	−0.7125
AH-7						AH-8				
298.15	1.3336	1.3296	0.3022	1.3298	0.2872	0.2025	0.2017	0.4147	0.2070	−2.1527
303.15	1.3580	1.3613	−0.2430	1.3613	−0.2430	0.2356	0.2391	−1.4856	0.2388	−1.3158
308.15	1.3834	1.3925	−0.6585	1.3925	−0.6585	0.2788	0.2788	0.0215	0.2742	1.6711
313.15	1.4210	1.4235	−0.1759	1.4234	−0.1689	0.3240	0.3201	1.2037	0.3135	3.2716
318.15	1.4541	1.4540	0.0096	1.4540	0.0096	0.3593	0.3622	−0.7959	0.3569	0.7069
323.15	1.4912	1.4843	0.4647	1.4843	0.4647	0.4023	0.4041	−0.4474	0.4046	−0.5469
328.15	1.5125	1.5114	0.0707	1.5142	0.0707	0.4454	0.4452	0.0427	0.4570	−2.5843
1-pentanol										
AH-1						AH-2				
298.15	0.2265	0.2251	0.6181	0.2366	4.4592	0.2566	0.2589	−0.8924	0.2796	−8.9981
303.15	0.2740	0.2733	0.2555	0.2731	0.2920	0.3320	0.3298	0.6627	0.3287	0.9639
308.15	0.3123	0.3232	−3.5002	0.3139	−0.5220	0.4065	0.4037	0.6839	0.3845	5.3582
313.15	0.3810	0.3727	2.1785	0.3591	5.7218	0.4750	0.4759	−0.1895	0.4476	5.7474
318.15	0.4268	0.4198	1.6355	0.4091	4.1192	0.5352	0.5414	−1.1622	0.5184	3.0980
323.15	0.4570	0.4626	−1.2254	0.4642	−1.6193	0.5920	0.5957	−0.6250	0.5978	−1.0135
328.15	0.4987	0.4991	−0.0722	0.5247	−5.2452	0.6391	0.6354	16.2312	0.6864	−7.4256
AH-3						AH-4				
298.15	0.2535	0.2534	0.0513	0.2579	−1.7237	0.3104	0.3099	0.1579	0.3153	−0.8731
303.15	0.2750	0.2865	−4.1818	0.2855	−3.8182	0.3300	0.3324	−0.7273	0.3340	−0.6970
308.15	0.3039	0.3199	−5.2407	0.3150	−3.6287	0.3542	0.3542	0.0028	0.3531	0.6522
313.15	0.3540	0.3530	0.2825	0.3464	2.1186	0.3749	0.3750	−0.0267	0.3727	0.8002
318.15	0.3875	0.3853	0.5575	0.3799	1.9512	0.3951	0.3947	0.0962	0.3927	0.6530
323.15	0.4235	0.4161	1.7473	0.4154	1.8890	0.4120	0.4133	−0.3155	0.4130	−0.3398

(*continued on next page*)

Table 2 (*continued*)

$T(K)$	$x_i \cdot 10^3$	$x_{ci}{}^a \cdot 10^3$	$100 \cdot RD^a$	$x_{ci}{}^b \cdot 10^3$	$100 \cdot RD^b$	$x_i \cdot 10^3$	$x_{ci}{}^a \cdot 10^3$	$100 \cdot RD^a$	$x_{ci}{}^b \cdot 10^3$	$100 \cdot RD^b$
328.15	0.4420	0.4451	−0.6945	0.4530	−2.5044	0.4298	0.4304	−0.1349	0.4338	−1.1819
AH-5						AH-6				
298.15	1.7575	1.7577	−0.0131	1.7579	−0.0131	0.3542	0.3531	0.3077	0.3497	1.2394
303.15	1.7830	1.7860	−0.1683	1.7861	−0.1683	0.4000	0.4003	−0.0750	0.4006	−0.1500
308.15	1.8109	1.8138	−0.1585	1.8139	−0.1585	0.4483	0.4539	−1.2605	0.4568	−1.9520
313.15	1.839	1.8412	−0.1196	1.8412	−0.1142	0.5100	0.5147	−0.9216	0.5188	−1.7451
318.15	1.8662	1.8680	−0.0965	1.8680	−0.0911	0.6000	0.5835	2.7500	0.5868	2.1667
323.15	1.8900	1.8943	−0.2275	1.8944	−0.2222	0.6900	0.6614	4.1449	0.6612	4.1449
328.15	1.9204	1.9201	0.0156	1.9203	0.0104	0.7400	0.7495	−1.2838	0.7423	−0.3378
AH-7						AH-8				
298.15	1.5587	1.5650	0.3022	1.5722	0.2872	0.2806	0.2816	−0.3411	0.2871	−2.3336
303.15	1.6220	1.6225	−0.2430	1.5832	−0.2430	0.3256	0.3260	0.1689	0.3248	0.2479
308.15	1.6834	1.6802	−0.6585	1.6395	−0.6585	0.3679	0.3704	−0.6983	0.3659	0.5347
313.15	1.7400	1.7381	−0.1759	1.6959	−0.1689	0.4236	0.4171	1.5361	0.4106	3.0564
318.15	1.7903	1.7959	0.0096	1.7524	0.0096	0.4551	0.4642	−2.0235	0.4591	−0.9111
323.15	1.8500	1.8539	0.4647	1.8089	0.4647	0.5130	0.5112	0.3448	0.5117	0.2483
328.15	1.9095	1.9118	0.0707	1.8655	0.0707	0.5572	0.5573	−0.0072	0.5683	−2.0056
Ethyl acetate										
AH-1						AH-2				
298.15	0.2412	0.2415	−0.1202	0.2387	1.9112	0.1590	0.1572	1.1507	0.1656	−4.1942
303.15	0.2564	0.2570	−0.2340	0.2571	−6.5523	0.1952	0.2020	−3.4836	0.2015	−3.2275
308.15	0.2739	0.2743	−0.1168	0.2763	−14.5700	0.2435	0.2518	−3.3916	0.2435	−0.0246
313.15	0.2923	0.2935	−0.4105	0.2963	−22.8870	0.3120	0.3051	2.2115	0.2926	6.1859
318.15	0.3166	0.3149	0.5495	0.3170	−29.2320	0.3621	0.3599	0.6076	0.3495	3.4521
323.15	0.3359	0.3386	−0.8038	0.3384	−38.2260	0.4030	0.4142	−2.7792	0.4152	−3.0521
328.15	0.3650	0.3649	0.0301	0.3606	−43.7770	0.4625	0.4656	−0.6768	0.4907	−6.1258
AH-3						AH-4				
298.15	0.2567	0.2543	0.9620	0.2566	0.0662	0.3554	0.3588	−0.9453	0.3684	−3.6462
303.15	0.2900	0.2934	−1.1724	0.2932	−1.1035	0.4250	0.4081	3.9765	0.4076	4.1176
308.15	0.3282	0.3356	−2.2641	0.3335	−1.6242	0.4713	0.4571	3.0047	0.4495	4.6386
313.15	0.3850	0.3808	1.0909	0.3779	1.8442	0.5200	0.5046	2.9615	0.4941	5.0000
318.15	0.4323	0.4288	0.8188	0.4265	1.3508	0.5545	0.5497	0.8710	0.5416	2.3497
323.15	0.4820	0.4794	0.5394	0.4795	0.5187	0.5900	0.5912	−0.2034	0.5920	−0.3051
328.15	0.5265	0.5325	−1.1492	0.5373	−2.0610	0.6291	0.6284	0.1033	0.6452	−2.5515
AH-5						AH-6				
298.15	1.4902	1.4878	0.1604	1.4879	0.1604	0.7700	0.7820	−1.5584	0.8160	−5.9610
303.15	1.5220	1.5269	−0.3219	1.5269	−0.3154	0.9500	0.9263	2.4947	0.9246	2.6842
308.15	1.5618	1.5656	−0.2459	1.5656	−0.2395	1.0670	1.0719	−0.4592	1.0434	2.2212
313.15	1.6000	1.6041	−0.2563	1.6040	−0.2438	1.2000	1.2134	−1.1167	1.1730	2.2583
318.15	1.6407	1.6422	−0.0939	1.6421	−0.0817	1.3470	1.3456	0.1039	1.3138	2.4722
323.15	1.6809	1.6799	0.0595	1.6799	0.0714	1.4500	1.4635	−0.9310	1.4663	−1.1172
328.15	1.7150	1.7173	−0.1318	1.7174	−0.1318	1.5720	1.5629	0.5789	1.6311	−3.7532
AH-7						AH-8				
298.15	0.8095	0.8077	0.2236	0.8077	0.2112	1.3007	1.3030	−0.1745	1.3025	−0.1361
303.15	0.8260	0.8286	−0.3148	0.8285	−0.3027	1.4875	1.4912	−0.2487	1.4911	−0.2420
308.15	0.8463	0.8492	−0.3486	0.8491	−0.3486	1.6977	1.6993	−0.0954	1.6996	−0.1131
313.15	0.8680	0.8696	−0.1843	0.8696	−0.1959	1.9423	1.9287	0.7002	1.9292	0.6745
318.15	0.8862	0.8899	−0.4221	0.8899	−0.4221	2.1658	2.1807	−0.6889	2.1811	−0.7074
323.15	0.9100	0.9100	0.0000	0.9100	0.0000	2.4368	2.4566	−0.8125	2.4565	−0.8084
328.15	0.9352	0.9299	0.5646	0.9299	0.5646	2.7694	2.7578	0.4196	2.7567	0.4593
Acetonitrile										
AH-1						AH-2				
298.15	0.0291	0.0290	0.2751	0.0325	−11.761	0.0571	0.0568	0.5428	0.0568	0.5428
303.15	0.0416	0.0423	−1.8252	0.0421	−0.8646	0.0650	0.0661	−1.6923	0.0661	−1.8462
308.15	0.0587	0.0581	0.9193	0.0540	8.0695	0.0761	0.0766	−0.7232	0.0766	−0.7232
313.15	0.0762	0.0754	0.9576	0.0687	9.8780	0.0930	0.0882	5.1613	0.0883	5.0538
318.15	0.0921	0.0927	−0.8686	0.0868	5.7546	0.1017	0.1013	0.3835	0.1013	0.3835
323.15	0.1109	0.1083	2.0739	0.1089	1.8034	0.1200	0.1157	3.5833	0.1157	3.5000
328.15	0.1218	0.1209	0.6568	0.1357	−11.494	0.1325	0.1317	0.6263	0.1317	0.6263
AH-3						AH-4				
298.15	0.1162	0.1172	−0.8432	0.1211	−4.1129	0.1131	0.1146	−1.3711	0.1170	−3.4056
303.15	0.1350	0.1347	0.2222	0.1345	0.4444	0.1350	0.1327	1.7037	0.1326	1.8519
308.15	0.1535	0.1521	0.9379	0.1489	3.0871	0.1519	0.1517	0.1054	0.1497	1.4882
313.15	0.1712	0.1688	1.4191	0.1643	4.1056	0.1700	0.1712	−0.7059	0.1684	1.0000
318.15	0.1824	0.1842	−0.9758	0.1807	0.9429	0.1889	0.1909	−1.0267	0.1887	0.1905
323.15	0.1930	0.1980	−2.5907	0.1982	−2.6943	0.2100	0.2105	−0.2381	0.2107	−0.2857
328.15	0.2112	0.2097	0.7008	0.2168	−2.6139	0.2304	0.2296	0.3645	0.2344	−1.6751
AH-5						AH-6				
298.15	0.7521	0.7624	−1.3735	0.7614	−1.2406	0.0178	0.0206	−15.7300	0.0526	−75.8430
303.15	0.8020	0.8043	−0.2868	0.8033	−0.1496	0.0600	0.0488	18.6667	0.0709	20.1667
308.15	0.8574	0.8471	1.2071	0.8460	1.3354	0.1010	0.0943	6.6337	0.0947	28.3168
313.15	0.8900	0.8906	−0.0674	0.8895	0.0562	0.1400	0.1507	−7.6429	0.1252	22.8571
318.15	0.9431	0.9350	0.8589	0.9338	0.9861	0.1870	0.2012	−7.5936	0.1642	14.9198
323.15	0.9700	0.9800	−1.0309	0.9788	−0.9072	0.2100	0.2272	−8.1905	0.2134	−10.2860
328.15	1.0107	1.0258	−1.4960	1.0245	89.8583	0.2410	0.2190	9.1286	0.2752	−38.0910

Table 2 (*continued*)

$T(K)$	$x_i \cdot 10^3$	$x_{ci}^a \cdot 10^3$	$100 \cdot RD^a$	$x_{ci}^b \cdot 10^3$	$100 \cdot RD^b$	$x_i \cdot 10^3$	$x_{ci}^a \cdot 10^3$	$100 \cdot RD^a$	$x_{ci}^b \cdot 10^3$	$100 \cdot RD^b$
AH-7						AH-8				
298.15	0.1647	0.1660	−0.7648	0.1717	−4.2248	0.1026	0.1031	−0.4873	0.1063	−3.5838
303.15	0.2001	0.1948	2.6487	0.1945	2.7986	0.1230	0.1235	−0.4065	0.1231	−0.0342
308.15	0.2274	0.2244	1.3323	0.2195	3.5308	0.1476	0.1450	1.7615	0.1418	3.9451
313.15	0.2500	0.2536	−1.4400	0.2466	1.3600	0.1633	0.1672	−2.4330	0.1627	0.4127
318.15	0.2823	0.2816	0.2586	0.2761	2.2066	0.1897	0.1896	0.0659	0.1858	2.0880
323.15	0.3010	0.3077	−2.2259	0.3081	−2.3588	0.2156	0.2113	1.9694	0.2113	2.0102
328.15	0.3291	0.3309	−0.5592	0.3426	−4.1148	0.2323	0.2320	0.2494	0.2394	−2.9067

(x_i) = Experimental mole fraction solubility with an uncertainty of ±0.00001.
[a] Values obtained by Apelblat equation (Eq. (2)).
[b] Values obtained by Buchowski-Ksiazczak equation (Eq. (3)).

Overall, eight compounds are synthesized and the IUPAC names of these compounds are:

AH-1:(E)-1-(1H-benzo[d] imidazole-2-yl)-3-(3-methxyphenyl-1H-pyrazol-4-yl)prop-2-en1one

AH-2:(E)-1-(1H-benzo[d]imidazole-2-yl)-3-(1, 3-diphenyl-1H-pyrazol-4-yl) prop-2-en-1one

AH-3:(E)-1-(1H-benzo[d] imidazole-2-yl)-3-(3-(4-chlorophenyl)-phenyl-1H-pyrazol-4-yl) prop-2-en-1one

AH-4:(E)-1-(1H-benzo[*d*] imidazole-2-yl)-3-(3-(3,4-dimethoxyphenyl)-1-phenyl-1H-pyrazol-4-yl) prop-2-en-1one

AH-5:(E)-1-(1H-benzo[*d*] imidazole-2-yl)-3-(3-(4-fluorophenyl)-1H-pyrazol-4-yl)pop-2-en-1one

AH-6:(E)-1-(1H-benzo[d]imidazole-2-yl)-3-(3-(2-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl) prop-2-en-1one

AH-7:(E)-1-(1H-benzo[*d*] imidazole-2-yl)-3-(3-(4-methxyphenyl)-1-phenyl-1H-pyrazol-4-yl) prop-2-en-1one

AH-8: (E)-1-(1H-benzo[*d*] imidazole-2-yl)-3-(3-(3-nitrophenyl)-1-phenyl-1H-pyrazol-4-yl) prop-2-en-1one

Table 1 shows the physical parameters and different substitutions of synthesized compounds.

2.2. Spectroscopy studies

The structure confirmation was done by different spectroscopic techniques such as IR, ^{1}H NMR, ^{13}CNMR and mass.

3. Solubility measurement

The isothermal saturation method [20] was used to determine the solubility of compounds. For each measurement, an excess amount of compound was added to known volume of selected solvent at a definite temperature. The desired temperature was controlled by the thermostatic water bath (Model No. 140285, Nova, India) and had a standard uncertainty of ±0.05 K. A magnetic stirrer was used to mix the solution. The solutions were stirred for few hours to reach solid-liquid equilibrium. The stirring was then stopped and the mixture was allowed to settle so that undissolved compound should be completely settled at the bottom. From this saturated solution, 5 ml of clear saturated solution was quickly withdrawn from the pre-heated or pre-cooled syringe from the solution and taken in a vial which had been weighed before (m_0). The vial with the saturated solution was then immediately weighted (m_1) to determine the weight of sample solution (m_1-m_0). The solvent of the solution in the vial was then allowed to evaporate at room temperature (about 35 °C) for at least 48 h. For some solvents, it may take longer. When all the solvent is evaporated, the weight of vial was again taken (m_2) to determine the weight of dry residue compound (m_2-m_0). This weight should be again taken after 24 h. If there is decrease in weight it suggests that solvent is not completely evaporated. So, more evaporation time should be given. This should continue until the weight was constant. The total evaporation of solvent was further confirmed by comparing TG of residue with that of original compound. At each temperature experiment was conducted three times in parallel and the average value was used as experimental result to calculate the mole solubility of compound. An analytical balance (Mettler Toledo AB204-S, Switzerland) was employed to determine the mass of solute, solvent, and saturated solution with the accuracy of ±0.0001 g. The mole fraction solubility of the solute i.e., compound (x_{exp}) in different pure solvents can be calculated by the following relation:

$$x_i = \frac{\frac{(m_2 - m_0)}{M_2}}{\left(\frac{m_2 - m_o}{M_2}\right) + \left(\frac{m_1 - m_2}{M_1}\right)} \quad (1)$$

where M_1 and M_2 is the molecular weight of solvent and compound respectively. m_1 and m_2 are weights of solvent and compound in the solution respectively. At each temperature, the measurement was repeated three times and an average value is given in Table 2. The uncertainty of experimental values is established to be less than 1.03%.

3.1. Results and discussion

The experimental mole fraction solubilities (x_i) of the studied compounds in the selected solvents are listed in Table 2 at different temperatures. It is observed that for alcoholic solvent, solubility increases from methanol to 1-pentanol. Thus, in alcohols, as -CH_2- group increases, solubility increases. For each compound, in non-alcoholic solvents, solubility is higher in ethyl acetate than that in acetonitrile.

Table 3 shows dielectric constant, dipole moment and hydrogen bonding capacity of studied solvents. It is observed that in alcohols, there is a regular decrease in dielectric constant and δ_H (Hydrogen bonding capacity) from methanol to 1-pentanol i.e., with increases in -CH_2- group. However, dipole moment is not in a systematic order. Thus, solubility in alcohols is reverse of dielectric constant and hydrogen bonding capacity.

For non-alcoholic solvents, all these three parameters are higher in acetonitrile than those for ethyl acetate. So, solubility in alcohols is reverse of these parameters i.e., dielectric constant, dipole moment and hydrogen bonding capacity.

It is also observed that different compounds have different solubility in a particular solvent. This is due to different types of interactions taking place in solution due to different substitution groups present in compounds. As shown in Table 1, all the studied compounds have same central moiety but different side chain substitutions which are of different nature. The solubility of AH-5 is maximum in all selected solvents. AH-1 has minimum solubility in methanol, ethyl acetate and acetonitrile. In 1-propanol, 1-butanol and 1-pentanol, AH-3 had minimum solubility whereas AH-4 was minimum soluble in ethanol.

Table 3
Dielectric constant, dipole moment and hydrogen bond capacity of studied solvents at 293.15 K.

Solvent	Dielectric constant	Dipole moment	δ_H Hydrogen bonding
Methanol	33.00	1.70	29.60
Ethanol	25.30	1.69	26.30
1-propanol	20.80	1.55	24.30
1-butanol	17.84	1.66	23.30
1-pentanol	15.30	1.70	22.30
Ethyl acetate	6.08	1.78	18.60
Acetonitrile	37.50	3.93	24.30

It is also observed that different compounds have different solubility in a particular solvent. The solubility of AH-5 is maximum in all selected solvents. AH-1 has minimum solubility in methanol, ethyl acetate and acetonitrile. The different solubility of compounds in different solvents may be due to different types of interactions taking place in solution due to different substitution groups present in compounds. As shown in Table 1, all the studied compounds have same central moiety but different side chain substitutions which are of different nature. Thus, different side substitution and orientation of compounds play important role in solubility. Table 1 also shows the electronegativity of different substitutions. The highest electronegativity is for flouro group present in AH-5. It is observed that AH-5 exhibited maximum solubility in all the solvents except ethyl acetate. However, for the other compounds, the electronegativity order of order of substitution is not always observed. This may be due to the fact that different substitutions interact differently with different solvents thus, affecting solubility of compounds in different solvents.

As temperature increases solubility increases and the trend of solubility of compounds in different solvents changed. The temperature dependence of solubility of compounds is described by the modified Apelblat model [21].

$$\ln x_{ci}^{a} = A + \frac{B}{T} + C\ \ln T \tag{2}$$

where T is the experimental temperature and A, B and C are parameters determined by least square method. The values of these parameters are listed in Table 4 for all the compounds. Using these parameters, mole fraction solubility (x^{a}_{ci}) was evaluated and is given in Table 2.

To describe solid-liquid equilibrium, Buchowski et al. [22] introduced a new model known as Buchowski-Ksiazczak (λh) model by

Table 4
Parameters of modified Apelblat equation, RMSD and ARD in the studied solvents.

Parameters	AH-1	AH-2	AH-3	AH-4	AH-5	AH-6	AH-7	AH-8
Methanol								
A	114.88	377.28	746.80	135.15	−5.11	415.30	−5.33	261.34
B	−7886.10	−284.60	−37,947.20	−8721.70	−385.98	−21,871.30	−714.14	−14,471.80
C	−17.3658	−56.1135	−110.5077	−20.4103	−0.1892	−61.6457	−0.1942	−39.1236
10^3*RMSD*	0.2529	2.2106	38.5458	1.4814	2.1551	3.0832	1.1013	1.5201
100 ARD	−0.0058	−0.2359	8.0509	−0.7801	−0.2363	−0.1614	−0.4140	−0.8047
Ethanol								
A	261.58	129.48	−4.21	352.81	−4.97	286.98	−4.71	−116.65
B	−25,849.80	−8213.83	−1708.24	−19,714.90	−350.88	−15,660.19	−819.05	2804.80
C	−74.2105	−19.5383	0.1299	−52.1000	−0.1696	−42.7569	−0.0853	17.1016
10^3*RMSD*	2.1042	1.5096	23.3510	1.5096	1.7205	39.5064	2.6843	1.8610
100 ARD	−0.8806	−0.2909	−0.4024	−0.2909	0.0316	−19.1956	−0.1289	−0.3108
1-propanol								
A	261.58	302.75	757.20	−3.77	−4.88	−121.90	−4.36	394.42
B	−14,356.80	−16,182.10	−37,401.00	−1766.16	−415.92	4035.40	−834.58	−20,814.80
C	−39.0361	−45.1755	−112.5295	0.1247	−0.1046	17.4818	−0.0788	−58.5647
10^3*RMSD*	2.5667	6.3069	20.7630	1.5822	7.3445	14.3387	4.1047	4.3743
100 ARD	0.5725	−1.8323	−0.2364	0.0957	0.1451	−2.4437	0.2828	−0.9019
1-butanol								
A	−3.69	−199.10	318.98	613.78	−4.77	91.84	−4.63	−277.55
B	−1930.54	7060.42	−17,024.30	−31,211.00	−232.00	−6274.82	−450.04	−15,439.50
C	0.2592	29.3312	−47.5087	−90.8846	−0.1570	−13.8547	−0.0843	−41.1189
10^3*RMSD*	2.0557	3.8434	17.8166	4.9127	7.5409	6.6894	5.2529	2.5569
100 ARD	−0.1412	0.1695	−3.7036	0.1768	0.0450	−0.4644	−0.0761	−0.2087
1-pentanol								
A	512.22	814.12	211.88	104.46	−4.63	−102.49	−4.19	206.73
B	−26,323.08	−40,587.73	−11,755.40	−6120.57	−323.03	2308.34	−656.99	−11,840.90
C	−75.8809	−120.4449	−31.7217	−16.1489	−0.1108	15.2351	−0.0127	−30.7487
10^3*RMSD*	6.7208	42.4911	8.7167	1.1677	2.7065	14.3513	4.2038	4.7972
100 ARD	−0.1040	2.2287	−1.0756	−0.1579	−0.1078	0.4792	−0.0538	−0.0970
Ethyl acetate								
A	−2.23	556.45	97.63	277.20	−4.51	450.18	−4.81	−2.23
B	−2270.08	−29,186.30	−6944.29	−14,758.80	−487.93	0.01	−495.25	−2270.07
C	18.3379	−82.0195	−14.4995	−41.3572	−0.0642	−66.6687	−0.1141	0.5613
10^3*RMSD*	1.4327	7.1356	4.9396	11.2528	3.4097	14.0017	3.2446	12.6234
100 ARD	−0.1408	−1.0732	−0.3052	1.5305	−0.1415	0.0958	−0.1007	−0.1037
Acetonitrile								
A	1228.64	−3.18	349.16	1.53	−3.97	4430.49	365.05	347.42
B	−61,362.30	−2620.72	−18,220.10	−12,436.60	−966.54	−212,352.00	−19,223.90	−18,763.00
C	−181.3525	0.3849	−52.1972	−32.5214	0.0047	−654.4960	−54.2817	−51.5424
10^3*RMSD*	1.1531	2.7074	2.5622	1.5208	10.1135	14.5724	4.0953	2.6276
100 ARD	0.2734	1.0484	−0.0409	0.0289	−0.1164	1.5717	0.0021	0.1724

Table 5
Parameters of Buchowski-Ksiazczak λh equation, RMSD and ARD in the studied solvents.

Parameters	AH-1	AH-2	AH-3	AH-4	AH-5	AH-6	AH-7	AH-8
Methanol								
$\lambda \cdot 10^2$	0.0759	0.2707	0.6404	0.0935	0.0928	0.4978	0.0382	0.1057
$h \cdot 10^4$	323.59	93.86	51.19	0.2353	35.19	52.17	170.88	211.72
10^3RMSD	0.3846	2.9194	4.3981	1.2374	2.0776	4.5131	1.0966	1.3851
100 ARD	−0.1195	−0.3285	−1.0174	−0.7756	−0.2266	−0.2277	−0.4059	−0.8413
Ethanol								
$\lambda \cdot 10^2$	0.2727	0.2505	0.1403	0.5686	0.1279	0.3541	0.1148	0.2134
$h \cdot 10^4$	97.04	89.51	124.61	0.3425	22.75	64.71	69.02	70,361.77
10^3RMSD	4.5802	7.4597	2.2568	7.4597	1.5086	3.3585	2.6828	1.6848
100 ARD	−0.0972	0.8131	−0.2997	0.8131	0.0329	0.1488	−0.1252	−0.4667
1-propanol								
$\lambda \cdot 10^2$	0.2360	0.3126	0.1681	0.0044	0.1873	0.1356	0.1645	0.4420
$h \cdot 10^4$	91.17	65.81	112.68	34,369.14	20.46	105.49	49.24	56.66
10^3RMSD	4.0335	6.3868	6.6333	0.0000	5.8225	4.1606	3.9687	5.2074
100 ARD	0.7852	−1.4112	0.5462	0.0000	0.0304	−1.1057	0.1958	−0.3340
1-butanol								
$\lambda \cdot 10^2$	0.2551	0.5878	533,474	0.9837	0.2103	0.5644	0.2494	0.8573
$h \cdot 10^4$	78.84	35.89	0.4068	32,059.67	8.69	34.42	16.99	30.13
10^3RMSD	2.0938	5.2158	7.8237	11.8787	7.5909	6.7426	5.2201	7.1468
100 ARD	−0.2698	−0.0539	−1.4706	0.9968	0.0407	−0.4655	−0.0750	0.1718
1-pentanol								
$\lambda \cdot 10^2$	0.7908	2.3484	0.4092	0.1418	0.2748	1.4508	0.4028	0.7114
$h \cdot 10^4$	32.86	12.47	44.90	1076.40	10.49	16.92	15.73	31.30
10^3RMSD	16.4757	26.8527	9.5826	3.1988	2.6542	13.9559	11.1608	7.7321
100 ARD	0.3924	0.9612	−0.57033	−0.0162	−0.1062	0.3038	−0.0554	0.1672
Ethyl acetate								
$\lambda \cdot 10^2$	0.1468	3.5151	0.9653	0.5173	0.3074	2.5194	0.1597	4.4241
$h \cdot 10^4$	91.65	94,201.48	24.98	35.34	15.22	8.98	28.76	5.53
10^3 RMSD	97.4333	16.1596	6.4183	18.5233	3.3239	38.5259	3.2309	12.7539
100 ARD	−22.1778	−0.3989	−0.1536	1.8928	−0.1344	0.6808	−0.1006	−0.1053
Acetonitrile								
$\lambda \cdot 10^2$	1.7668	0.3588	0.2111	0.3104	0.3426	18.9835	0.4887	0.4839
$h \cdot 10^4$	26.38	90,289.29	89.99	7.31	25.26	2.84	145,648.57	54.71
10^3RMSD	7.2925	2.6586	5.0919	2.7221	0.3708	44.4275	8.4498	4.6200
100 ARD	1.8781	0.9991	0.4674	0.3671	13.0256	5.4119	0.4889	0.7879

which solubility data can be correlated with temperature by the relation:

$$\ln\left(1+\frac{\lambda(1-x_{ci}^{b})}{x_{ci}^{b}}\right)=\lambda h\left[\frac{1}{T}-\frac{1}{T_m}\right] \tag{3}$$

where T and T_m are the experimental and melting temperature of compound. λ and h are two adjustable parameters. The values of λ and h are evaluated using experimental solubility data and are reported in Table 5. Using these values of adjustable parameters, solubility ($x^b{}_{ci}$) is calculated using Eq. (3) and obtained values are listed in Table 2.

The calculated solubility values by Apelblat and Buchowski-Ksiazczak (λh) models are also plotted against temperature in Figs. 2 to 5. It is observed that for all the compounds, there is good agreement between experimental solubility values with those evaluated ($x^b{}_{ci}$) by Apelblat model. However, when experimental solubility is compared with calculated values ($x^b{}_{ci}$) by Buchowski-Ksiazczak (λh) model, for some of the compounds, discrepancies are observed in some solvents. This indicates that for some solvents, Buchowski-Ksiazczak model is not suitable.

Comparison of solubility variation with temperature among different compounds suggest that when solubility various linearly with temperature, ($x^b{}_{ci}$) values evaluated by Buchowski-Ksiazczak (λh) model are in good agreement with experimental data but when variation of solubility with temperature is non-linear, ($x^b{}_{ci}$) deviates from experimental values.

This is further observed by relative deviation (*RD*), root-mean-square deviations (*RMSD*) and relative average deviations (*RAD*) which are calculated using following equations:

$$RD=\frac{\left(x_{exp}-x_{ci}^{a/b}\right)}{x_i} \tag{4}$$

$$RMSD=\left[\sum_{i=1}^{N}\frac{\left(x_{ci}^{a/b}-x_{exp}\right)^2}{N-1}\right]^{1/2} \tag{5}$$

$$RAD=\frac{1}{N}\sum_{i}^{N}\frac{\left(x_{exp}-x_{ci}^{a/b}\right)}{x_{exp}} \tag{6}$$

where x_{exp} is experimental solubility and $x^{a/b}{}_{ci}$ is calculated solubility. $x^a{}_{ci}$ and $x^b{}_{ci}$ are calculated solubility values from Apelblat and Buchowski–Ksiazczak models. N is the number of experimental points. The evaluated relative deviation (*RD*) values for both models are given in Table 2 where sroot-mean-square deviations (*RMSD*) and relative average deviations (*RAD*) values are listed in Tables 5 and 6 for both models.

It is evident from Table 2 that for some compounds, for some solvents, *RD* values for Buchowski-Ksiazczak model are higher than that evaluated for Apelblat model.

Table 6
Some thermodynamic parameters, ΔG_{sol}, ΔH_{sol} and ΔS_{sol} of dissolution of chalcone derivatives in the studied solvents.

Parameters	AH-1	AH-2	AH-3	AH-4	AH-5	AH-6	AH-7	AH-8
Methanol								
ΔG_{sol} $kJ \cdot mol^{-1}$	26.3 ± 0.2	24.3 ± 0.3	24.7 ± 0.04	26.0 ± 0.3	19.3 ± 0.5	44.5 ± 0.8	22.7 ± 0.3	25.3 ± 0.02
ΔH_{sol} $kJ \cdot mol^{-1}$	20.4 ± 0.2	21.1 ± 0.2	28.2 ± 0.4	19.4 ± 0.6	2.7 ± 0.2	21.0 ± 0.1	5.4 ± 0.6	18.6 ± 0.2
ΔS_{sol} $J \cdot mol^{-1}$	−18.8 ± 0.2	−10.2 ± 0.7	11.2 ± 0.8	−21.0 ± 0.2	−53.1 ± 0.6	−73.4 ± 0.7	−55.2 ± 0.03	−21.3 ± 0.6
Ethanol								
ΔG_{sol} $kJ \cdot mol^{-1}$	23.5 ± 0.8	23.5 ± 0.1	23.2 ± 0.2	24.9 ± 0.3	18.3 ± 0.8	22.7 ± 0.8	20.3 ± 0.5	24.4 ± 0.9
ΔH_{sol} $kJ \cdot mol^{-1}$	22.0 ± 0.1	17.5 ± 0.01	14.5 ± 0.4	28.47 ± 0.8	2.4 ± 0.8	19.0 ± 0.5	6.5 ± 0.9	21.1 ± 0.3
ΔS_{sol} $J \cdot mol^{-1}$	−5.0 ± 0.1	−19.2 ± 0.1	−27.7 ± 0.3	11.3 ± 0.6	−50.8 ± 0.4	−11.9 ± 0.3	−43.9 ± 0.8	−10.7 ± 0.2
1-propanol								
ΔG_{sol} $kJ \cdot mol^{-1}$	22.4 ± 0.1	22.2 ± 0.6	23.3 ± 0.1	22.6 ± 0.2	17.7 ± 0.3	22.1 ± 0.5	19.7 ± 0.7	22.4 ± 0.7
ΔH_{sol} $kJ \cdot mol^{-1}$	17.8 ± 0.9	17.1 ± 0.1	18.4 ± 0.4	15.0 ± 0.1	3.1 ± 0.9	11.8 ± 0.9	6.7 ± 0.3	20.8 ± 0.2
ΔS_{sol} $J \cdot mol^{-1}$	−14.4 ± 0.6	−16.4 ± 0.6	−15.5 ± 0.8	−24.3 ± 0.6	−46.4 ± 0.8	−32.8 ± 0.001	−40.7 ± 0.2	−5.2 ± 0.7
1-butanol								
ΔG_{sol} $kJ \cdot mol^{-1}$	21.7 ± 0.7	20.7 ± 0.9	21.9 ± 0.3	21.3 ± 0.09	16.6 ± 0.9	20.4 ± 0.6	17.0 ± 0.5	21.0 ± 0.1
ΔH_{sol} $kJ \cdot mol^{-1}$	16.7 ± 0.2	17.5 ± 0.4	18.0 ± 0.4	23.2 ± 0.4	1.5 ± 0.2	16.1 ± 0.5	3.5 ± 0.2	21.4 ± 0.8
ΔS_{sol} $J \cdot mol^{-1}$	−16.1 ± 0.5	−10.4 ± 0.02	−12.4 ± 0.04	5.9 ± 0.2	−48.5 ± 0.1	−13.7 ± 0.7	−43.2 ± 0.6	1.4 ± 0.9
1-pentanol								
ΔG_{sol} $kJ \cdot mol^{-1}$	20.6 ± 0.6	20.0 ± 0.8	20.7 ± 0.4	20.5 ± 0.6	16.3 ± 0.8	19.6 ± 0.9	16.5 ± 0.4	20.3 ± 0.04
ΔH_{sol} $kJ \cdot mol^{-1}$	21.6 ± 0.02	24.3 ± 0.6	15.2 ± 0.8	8.9 ± 0.1	2.3 ± 0.9	20.4 ± 0.1	5.4 ± 0.3	18.5 ± 0.2
ΔS_{sol} $J \cdot mol^{-1}$	3.0 ± 0.3	13.6 ± 0.6	−17.4 ± 0.7	−37.2 ± 0.2	−44.7 ± 0.1	2.2 ± 0.8	−35.5 ± 0.1	−5.7 ± 0.2
Ethyl acetate								
ΔG_{sol} $kJ \cdot mol^{-1}$	21.1 ± 0.5	21.1 ± 0.9	20.5 ± 0.2	19.8 ± 0.2	16.7 ± 0.4	17.7 ± 0.04	18.3 ± 0. 4	16.2 ± 0.8
ΔH_{sol} $kJ \cdot mol^{-1}$	11.1 ± 0.9	29.4 ± 0.5	20.0 ± 0.4	15.2 ± 0.01	3.8 ± 0.9	18.7 ± 0.8	3.8 ± 0.2	20.3 ± 0.3
ΔS_{sol} $J \cdot mol^{-1}$	−31.8 ± 0.3	26.3 ± 0.8	−1.5 ± 0.2	−14.7 ± 0.7	−41.0 ± 0.9	3.4 ± 0.5	−46.4 ± 0.02	12.9 ± 0.5
Acetonitrile								
ΔG_{sol} $kJ \cdot mol^{-1}$	24.9 ± 0.7	24.3 ± 0.01	22.6 ± 0.8	22.6 ± 0.2	18.2 ± 0.8	23.8 ± 0.2	21.6292	22.6 ± 0.8
ΔH_{sol} $kJ \cdot mol^{-1}$	38.7 ± 0.5	22.7 ± 0.8	15.7 ± 0.9	18.8 ± 0.6	8.0 ± 0.5	64.2 ± 0.3	18.7256	20.7 ± 0.7
ΔS_{sol} $J \cdot mol^{-1}$	44.0 ± 0.6	−4.8 ± 0.5	−22.0 ± 0.1	−12.0 ± 0.3	−32.6 ± 0.9	129.1 ± 0.9	−9.2814	−6.1 ± 0.06

Comparison of root-mean-square deviations (*RMSD*) and relative average deviations (*ARD*) values for both models in Tables 4 and 5 again confirms that Apelblat model is better for all the compounds in all the studied solvents whereas Buchowski-Ksiazczak model exhibited discrepancies in some solvents for few compounds, the reason of which is not clear.

3.2. Thermodynamic parameters

The dissolution process in solid and liquid is a pseudo chemical reaction [23]. From the energy point of view, the thermodynamic properties of dissolution process are of great significance in the study of solution structures. Thus, using experimental solubility data of compounds in different solvents, some thermodynamics parameters such as dissolution enthalpy (ΔH_{sol}), Gibb's free energy of dissolution (ΔG_{sol}) and entropy (ΔS_{sol}) have been evaluated. The following modified Van't Hoff equation [24] was used to calculate enthalpy of dissolution (ΔH_{sol}):

$$\left(\frac{\partial \ln x_{exp}}{\partial\left(\frac{1}{T}-\frac{1}{T_{hm}}\right)}\right)_p = -\frac{\Delta H_{sol}}{R} \tag{7}$$

where T is the experimental temperature, R is universal gas constant (= 8.314 J/mol K). T_{hm} is mean harmonic temperature [25] which is calculated by the following equation:

$$T_{hm} = \frac{n}{\sum_{i=1}^{n}\left(\frac{1}{T}\right)} \tag{8}$$

where n is the number of experimental temperatures studied. In the present study, the value of T_{hm} is 312.83 K.

Using Eq. (7), dissolution enthalpy was evaluated from the slope of the plot of ln x_{exp} versus $(1/T\text{-}1/T_{hm})$ for all the compounds in different solvents. The Gibb's free energy of dissolution was calculated by the intercept of these plots by the relation:

$$\Delta G_{sol} = -R.T_{hm}.Intercept \tag{9}$$

The entropy of dissolution (ΔS_{sol}) was evaluated by the following equation [26]:

$$\Delta S_{sol} = \frac{(\Delta H_{sol} - \Delta G_{sol})}{T_{hm}} \tag{10}$$

All these thermodynamic parameters are given in Table 6. It is observed that for all the compounds, enthalpy (ΔH_{sol}) and Gibb's free energy of dissolution (ΔG_{sol}) are positive. The entropy values are both positive and negative for different compounds in different solvents.

The positive enthalpy (ΔH_{sol}) indicates that dissolution of studied compounds in selected solvents is endothermic process. As mentioned above, presence of different groups interact differently with solvent molecules. However, these interactions are stronger than intramolecular interactions of compounds. Thus, these powerful interaction between compounds and solvent molecules results in positive enthalpy. The positive Gibb's free energy of dissolution (ΔG_{sol}) suggests spontaneous dissolution of compounds. The negative entropy is due to more order in solutions whereas positive entropy suggests more randomness in solution. Further, comparison of enthalpy of different compounds shows that in all the studied solvents, AH-5 exhibited minimum enthalpy whereas its solubility is maximum in all the studied solvents. However, there is no systematic correlation between solubility and Gibb's free energy and entropy. Again, due to different type and magnitude of interactions, thermodynamic parameters vary for different compounds due to different nature of substitution groups.

In Buchowski-Ksiazczak (λh) model, the parameter λ denotes the average value of the associative amount of solute molecules in a solute i.e., compound. Table 5 shows that values of λ are very small in studied solvents for all the compounds. This suggests that there is no obvious association formed during dissolution process.

Table 7
The relative contribution by enthalpy and entropy derived from thermodynamic data.

Parameters	AH-1	AH-2	AH-3	AH-4	AH-5	AH-6	AH-7	AH-8
Methanol								
$\%\xi_{TS}$	22.3	13.2	11.1	25.3	86.0	51.6	76.0	26.4
$\%\xi_H$	77.6	86.8	88.9	74.7	14.0	48.4	24.0	73.6
Ethanol								
$\%\xi_{TS}$	6.6	25.6	37.4	11.1	86.5	16.4	67.6	13.7
$\%\xi_H$	93.4	74.4	62.6	88.91	13.5	83.6	32.4	86.3
1-propanol								
$\%\xi_{TS}$	20.2	23.1	20.9	33.7	82.0	46.3	65.4	7.3
$\%\xi_H$	79.8	76.9	79.1	66.3	18.0	53.7	34.6	92.7
1-butanol								
$\%\xi_{TS}$	23.2	15.6	17.7	7.4	90. 9	21.1	79.3	2.1
$\%\xi_H$	76.8	84.4	82.3	92.6	9.1	78.9	20.7	97.9
1-pentanol								
$\%\xi_{TS}$	4.2	14.9	26.4	56.7	85.4	3.4	67.2	8.8
$\%\xi_H$	95.2	85.1	73.6	43.3	14.6	96.6	32.8	91.2
Ethyl acetate								
$\%\xi_{TS}$	47.1	21.9	2.3	23.3	76.8	5.4	79.2	16.6
$\%\xi_H$	52.9	78.1	97.7	76.7	23.2	94.6	20.8	83.4
Acetonitrile								
$\%\xi_{TS}$	26.2	6.2	30.4	16.6	56.0	38.6	13.4	8.4
$\%\xi_H$	73.8	93.8	69.6	83.3	44.0	61.4	86.6	91.6

The contribution of enthalpy and entropy to standard Gibb's energy of dissolution is also evaluated using the following equations [27]:

$$\%\xi_H = \frac{|\Delta H_{sol}|}{|\Delta H_{sol}| + |T.\Delta S_{sol}|}.100 \tag{11}$$

$$\%\xi_S = \frac{|T.\Delta S_{sol}|}{|\Delta H_{sol}| + |T.\Delta S_{sol}|}.100 \tag{12}$$

The ξ_H and ξ_{TS} represent the comparison of relative contribution to the standard Gibbs energy by enthalpy and entropy towards the solution process, respectively. These values are listed in Table 7. The comparison of these evaluated contributions of enthalpy and entropy to solubility does not give systematic order.

Among alcohols, only for compounds AH-5, AH-7 and AH-6, solubility is reverse of ξ_H. For other compounds, in both alcoholic and non-alcoholic solvents, no regular trend is observed. However, in almost all the cases, the main contributor to standard Gibbs energy of solution is enthalpy during the dissolution because the values of $\%\xi_H$ are greater than 50%. The ξ_H and ξ_{TS} values are different for different compounds in different solvents. It is observed that in alcohols, for all the solvents, highest enthalpy of contribution is for AH-3 in methanol, AH-1 in ethanol, AH-1 in 1-propanol, AH-8 in 1-butanol, AH-6 in 1-pentanol, AH-3 in ethyl acetate and AH-2 in acetonitrile. However, entropy of contribution is higher for AH-5 in all the alcohols. Further, comparison of these evaluated contributions of enthalpy and entropy to electro negativity of substitutions (Table 1) does not give any systematic order.

The net variation in enthalpy results from the contribution of several kinds of interactions such as ion-dipole, vander Waals, Lewis acid-base interactions etc. [28]. The synthesized compounds could act as Lewis base in solutions due to the presence of free electron pairs on carbonyl and secondary amine groups (Fig. 1). These compounds may form hydrogen bonding with proton acceptor groups present in the solvents. Otherwise, these compounds could also act as Lewis acid because the proton on its secondary group present on benzo [d] imidazole ring may interact with the free electron pair of oxygen present in most of the studied solvents [29]. Thus, more deep research is required to understand the possible mechanism involved in the dissolution of studied compounds.

The apparent dissolution enthalpy ΔH_{sol} can be derived from the Gibbs-Helmholtz equation [30] and the modified Apelblat equation, and then expressed as following equation

$$\Delta H_{sol} = R(-B + CT) \tag{13}$$

where B and C are parameters of modified Apelblat equation represented in Table 4, R is the universal gas constant ($8.314\ J\cdot K^{-1}\cdot mol^{-1}$), and T is the absolute temperature.

The evaluated values are listed in Table 8. Comparison of enthalpy values reported in Tables 6 and 8 shows that either of two equations (Eqs. (7) and (13)) can be used for the evaluation of enthalpy. By Eq. (7), only one value of enthalpy was evaluated from the slope of the plot whereas by Eq. (13), at each temperature, enthalpy can be calculated.

The enthalpy of mixing is the enthalpy liberated or absorbed from a substance upon mixing [31]. When a substance or compound is combined with any other substance or compound the enthalpy of mixing is the consequence of the new interactions between the two substances or compounds. This enthalpy if released exothermically can in an extreme case cause an explosion.

Table 8
The apparent molar dissolution derived from thermodynamics data using Eq. (13).

Temp (K)	Methanol	Ethanol	1-propanol	1-butanol	1-pentanol	Ethyl acetate	Acetonitrile
ΔH_{sol} / (kJ·mol^{-1})							
AH-1							
298.15	22.5 ± 0.2	30.9 ± 0.6	22.5 ± 0.9	16.6 ± 0.9	30.7 ± 0.5	8.9 ± 0.8	60.6 ± 0.3
303.15	21.7 ± 0.2	27.8 ± 0.2	20.9 ± 0.8	16.7 ± 0.04	27.6 ± 0.06	9.7 ± 0.4	53.0 ± 0.8
308.15	21.0 ± 0.7	24.7 ± 0.9	19.3 ± 0.5	16.7 ± 0.1	24.4 ± 0.5	10.5 ± 0.002	45.5 ± 0.5
313.15	20.3 ± 0.5	21.7 ± 0.1	17.7 ± 0.3	16.7 ± 0.3	21.2 ± 0.9	11.2 ± 0.6	38.0 ± 0.1
318.15	19.6 ± 0.3	18.6 ± 0.2	16.1 ± 0.1	16.7 ± 0.4	18.1 ± 0.3	12.0 ± 0.2	30.4 ± 0.7
323.15	18.9 ± 0.1	15.5 ± 0.3	14.4 ± 0.9	16.7 ± 0.5	14.9 ± 0.8	12.7 ± 0.9	22.9 ± 0.3
328.15	18.1 ± 0.9	12.4 ± 0.5	12.8 ± 0.7	16.7 ± 0.6	11.8 ± 0.3	13.5 ± 0.5	15.3 ± 0.9
AH-2							
298.15	27.8 ± 0.9	19.8 ± 0.6	22.5 ± 0.6	15.8 ± 0.1	38.8 ± 0.9	39.3 ± 0.4	22.7 ± 0.4
303.15	25.5 ± 0.6	19.0 ± 0.5	20.6 ± 0.8	15.9 ± 0.5	33.8 ± 0.8	35.9 ± 0.3	22.7 ± 0.6
308.15	23.2 ± 0.2	18.2 ± 0.3	18.7 ± 0.9	16.0 ± 0.9	28.8 ± 0.7	32.5 ± 0.2	22.7 ± 0.7
313.15	20.8 ± 0.9	17.4 ± 0.2	16.9 ± 0.2	16.2 ± 0.5	23.8 ± 0.7	29.1 ± 0.1	22.7 ± 0.9
318.15	18.5 ± 0.6	16.6 ± 0.1	15.0 ± 0.4	16.3 ± 0.9	18.8 ± 0.6	25.7 ± 0.1	22.8 ± 0.1
323.15	16.2 ± 0.3	15.7 ± 0.9	13.1 ± 0.7	16.5 ± 0.4	13.8 ± 0.5	22.2 ± 0.9	22.8 ± 0.2
328.15	13.8 ± 0.9	14.9 ± 0.8	11.2 ± 0.9	16.6 ± 0.9	8.8 ± 0.4	18.8 ± 0.9	22.8 ± 0.3
AH-3							
298.15	41.5 ± 0.6	14.5 ± 0.2	32.0 ± 0.1	23.7 ± 0.7	19.1 ± 0.02	21.7 ± 0.9	22.0 ± 0.9
303.15	36.9 ± 0.7	14.5 ± 0.3	27.3 ± 0.3	21.7 ± 0.9	17.7 ± 0.8	21.1 ± 0.9	19.9 ± 0.3
308.15	32.3 ± 0.7	14.5 ± 0.3	22.6 ± 0.6	19.8 ± 0.2	16.4 ± 0.6	20.5 ± 0.8	17.7 ± 0.6
313.15	27.7 ± 0.8	14.5 ± 0.4	17.9 ± 0.8	17.8 ± 0.5	15.1 ± 0.5	19.9 ± 0.8	15.5 ± 0.9
318.15	23.1 ± 0.9	14.5 ± 0.5	13.3 ± 0.01	15.8 ± 0.7	13.8 ± 0.3	19.3 ± 0.8	13.4 ± 0.2
323.15	18.5 ± 0.9	14.5 ± 0.5	8.6 ± 0.2	13.9 ± 0.0	12.5 ± 0.1	18.7 ± 0.8	11.2 ± 0.5
328.15	14.0 ± 0.01	14.5 ± 0.6	3.9 ± 0.4	11.9 ± 0.3	11.1 ± 0.9	18.1 ± 0.7	9.0 ± 0.8
AH-4							
298.15	21.9 ± 0.2	34.7 ± 0.6	14.9 ± 0.9	34.2 ± 0.01	10.8 ± 0.6	20.1 ± 0.8	22.7 ± 0.8
303.15	21.0 ± 0.1	32.5 ± 0.9	14.9 ± 0.9	30.4 ± 0.2	10.1 ± 0.8	18.4 ± 0.7	21.4 ± 0.3
308.15	20.2 ± 0.2	30.4 ± 0.3	15.0 ± 0.03	26.6 ± 0.5	9.5 ± 0.1	16.7 ± 0.5	20.0 ± 0.8
313.15	19.3 ± 0.7	28.2 ± 0.7	15.0 ± 0.1	22.8 ± 0.7	8.8 ± 0.4	15.0 ± 0.2	18.7 ± 0.3
318.15	18.5 ± 0.2	26.1 ± 0.001	15.0 ± 0.1	19.0 ± 0.9	8.1 ± 0.7	13.3 ± 0.1	17.3 ± 0.7
323.15	17.6 ± 0.8	23.9 ± 0.3	15.0 ± 0.1	15.3 ± 0.1	7.4 ± 0.9	11.5 ± 0.9	16.0 ± 0.2
328.15	16.8 ± 0.3	21.7 ± 0.6	15.0 ± 0.2	11.5 ± 0.3	6.8 ± 0.3	9.8 ± 0.7	14.6 ± 0.7
AH-5							
298.15	2.7 ± 0.4	2.4 ± 0.9	3.1 ± 0.9	1.5 ± 0.4	2.4 ± 0.1	3.8 ± 0.9	8.0 ± 0.4
303.15	2.7 ± 0.3	2.4 ± 0.9	3.1 ± 0.9	1.5 ± 0.3	2.4 ± 0.1	3.8 ± 0.9	8.0 ± 0.5
308.15	2.7 ± 0.2	2.4 ± 0.8	3.1 ± 0.8	1.5 ± 0.3	2.4 ± 0.1	3.8 ± 0.9	8.0 ± 0.5
313.15	2.7 ± 0.2	2.4 ± 0.8	3.1 ± 0.8	1.5 ± 0.2	2.3 ± 0.9	3.8 ± 0.9	8.0 ± 0.5
318.15	2.7 ± 0.1	2.4 ± 0.7	3.1 ± 0.8	1.5 ± 0.1	2.3 ± 0.9	3.8 ± 0.9	8.0 ± 0.5
323.15	2.7 ± 0.01	2.4 ± 0.6	3.1 ± 0.7	1.5 ± 0.1	2.3 ± 0.9	3.8 ± 0.8	8.0 ± 0.5
328.15	2.6 ± 0.9	2.4 ± 0.5	3.1 ± 0.7	1.5 ± 0.04	2.3 ± 0.8	3.8 ± 0.8	8.0 ± 0.5
AH-6							
298.15	29.0 ± 0.3	24.2 ± 0.04	9.7 ± 0.8	17.8 ± 0.3	18.5 ± 0.7	26.8 ± 0.3	143.1 ± 0.2
303.15	26.4 ± 0.7	22.4 ± 0.3	10.5 ± 0.1	17.2 ± 0.5	19.2 ± 0.1	24.0 ± 0.5	115.9 ± 0.1
308.15	23.9 ± 0.1	20.6 ± 0.5	11.2 ± 0.3	16.6 ± 0.7	19.8 ± 0.4	21.2 ± 0.8	88.7 ± 0.02
313.15	21.3 ± 0.4	18.8 ± 0.7	11.9 ± 0.6	16.0 ± 0.9	20.4 ± 0.7	18.5 ± 0.1	61.4 ± 0.9
318.15	18.7 ± 0.8	17.0 ± 0.9	12.6 ± 0.9	15.5 ± 0.2	21.1 ± 0.1	15.7 ± 0.4	34.2 ± 0.8
323.15	16.2 ± 0.2	15.3 ± 0.2	13.4 ± 0.2	14.9 ± 0.5	21.7 ± 0.4	12.9 ± 0.9	7.0 ± 0.8
328.15	13.6 ± 0.6	13.5 ± 0.4	14.1 ± 0.4	14.3 ± 0.7	22.3 ± 0.7	10.1 ± 0.9	−20.1 ± 0.2
AH-7							
298.15	5.4 ± 0.5	6.5 ± 0.9	6.7 ± 0.4	3.5 ± 0.3	5.4 ± 0.3	3.8 ± 0.3	25.2 ± 0.7
303.15	5.4 ± 0.5	6.5 ± 0.9	6.7 ± 0.4	3.5 ± 0.3	5.4 ± 0.3	3.8 ± 0.3	23.0 ± 0.1
308.15	5.4 ± 0.4	6.5 ± 0.9	6.7 ± 0.4	3.5 ± 0.3	5.4 ± 0.3	3.8 ± 0.3	20.7 ± 0.6
313.15	5.4 ± 0.3	6.5 ± 0.8	6.7 ± 0.3	3.5 ± 0.2	5.4 ± 0.3	3.8 ± 0.2	18.5 ± 0.03
318.15	5.4 ± 0.4	6.5 ± 0.8	6.7 ± 0.3	3.5 ± 0.2	5.4 ± 0.3	3.8 ± 0.2	16.2 ± 0.05
323.15	5.4 ± 0.2	6.5 ± 0.8	6.7 ± 0.3	3.5 ± 0.2	5.4 ± 0.3	3.8 ± 0.1	13.9 ± 0.9
328.15	5.4 ± 0.1	6.5 ± 0.7	6.7 ± 0.2	3.5 ± 0.1	5.4 ± 0.3	3.8 ± 0.1	11.7 ± 0.3
AH-8							
298.15	23.3 ± 0.3	19.0 ± 0.7	27.8 ± 0.8	26.4 ± 0.4	22.2 ± 0.2	25.2 ± 0.7	28.2 ± 0.3
303.15	21.7 ± 0.1	19.7 ± 0.8	25.4 ± 0.5	24.7 ± 0.3	20.9 ± 0.5	23.0 ± 0.1	26.0 ± 0.8
308.15	20.0 ± 0.8	20.4 ± 0.9	23.0 ± 0.1	23.0 ± 0.2	19.6 ± 0.7	20.7 ± 0.6	23.9 ± 0.4
313.15	18.4 ± 0.5	21.2 ± 0.05	20.5 ± 0.8	21.3 ± 0.1	18.3 ± 0.9	18.5 ± 0.03	21.8 ± 0.03
318.15	16.8 ± 0.3	21.9 ± 0.2	18.1 ± 0.4	19.6 ± 0.01	17.1 ± 0.1	16.2 ± 0.5	19.6 ± 0.6
323.15	15.2 ± 0.06	22.6 ± 0.3	15.7 ± 0.1	17.8 ± 0.9	15.8 ± 0.3	13.9 ± 0.9	17.5 ± 0.2
328.15	13.5 ± 0.8	23.3 ± 0.2	13.2 ± 0.8	16.1 ± 0.8	14.5 ± 0.6	11.7 ± 0.3	15.3 ± 0.7

Table 9
The excess of enthalpy derived from thermodynamics data using Eq. (14).

Temp(K)	Methanol	Ethanol	1-propanol	1-butanol	1-pentanol	Ethyl acetate	Acetonitrile
H^E / (kJ·mol^{-1})							
AH-1							
298.15	1.1 ± 0.3	0.9 ± 0.8	1.3 ± 0.5	9.6 ± 0.7	1.0 ± 0.2	1.0 ± 0.6	0.6 ± 0.2
303.15	1.2 ± 0.5	1.0 ± 0.8	1.4 ± 0.9	10.5 ± 0.03	1.1 ± 0.5	1.0 ± 0.9	0.7 ± 0.2
308.15	1.3 ± 0.7	1.2 ± 0.5	1.6 ± 0.5	11.9 ± 0.3	1.2 ± 0.5	1.1 ± 0.5	0.8 ± 0.5
313.15	1.5 ± 0.1	1.3 ± 0.7	1.81 ± 0.2	12.9 ± 0.3	1.4 ± 0.4	1. ± 0.9	0.9 ± 0.8
318.15	1.6 ± 0.4	1.4 ± 0.9	1.9 ± 0.6	14.4 ± 0.8	1.5 ± 0.6	1.2 ± 0.6	1.1 ± 0.001
323.15	1.7 ± 0.8	1.5 ± 0.9	2.1 ± 0.5	15.9 ± 0.5	1.6 ± 0.5	1.3 ± 0.2	1.2 ± 0.4
328.15	1.9 ± 0.6	1.7 ± 0.3	2.2 ± 0.5	17.3 ± 0.7	1.7 ± 0.6	1.3 ± 0.9	1.3 ± 0.3
AH-2							
298.15	0.5 ± 0.01	0.7 ± 0.9	0.8 ± 0.2	6.2 ± 0.2	0.3 ± 0.4	0.2 ± 0.1	0.5 ± 0.3
303.15	0.5 ± 0.8	0.8 ± 0.8	0.9 ± 0.1	6.8 ± 0.9	0.4 ± 0.2	0.2 ± 0.4	0.5 ± 0.9
308.15	0.7 ± 0.07	0.9 ± 0.8	1.0 ± 0.5	7.4 ± 0.9	0.4 ± 0.9	0.2 ± 0.8	0.6 ± 0.9
313.15	0.7 ± 0.7	1.1 ± 0.2	1.1 ± 0.1	8.3 ± 0.9	0.5 ± 0.7	0.3 ± 0.4	0.8 ± 0.2
318.15	0.8 ± 0.5	1.2 ± 0.2	1.2 ± 0.6	9.3 ± 0.6	0.6 ± 0.3	0.3 ± 0.8	0.8 ± 0.9
323.15	0.9 ± 0.8	1.3 ± 0.2	1.3 ± 0.1	10.6 ± 0.2	0.6 ± 0.9	0.4 ± 0.1	1.0 ± 0.3
328.15	1.0 ± 0.4	1.4 ± 0.3	1.4 ± 0.7	11.6 ± 0.2	0.7 ± 0.3	0.4 ± 0.6	1.1 ± 0.3
AH-3							
298.15	0.1 ± 0.8	1.0 ± 0.6	0.7 ± 0.9	5.5 ± 0.5	0.9 ± 0.6	0.5 ± 0.5	0.8 ± 0.8
303.15	0.2 ± 0.3	1.1 ± 0.8	0.9 ± 0.8	6.4 ± 0.5	1.0 ± 0.4	0.6 ± 0.2	1.0 ± 0.2
308.15	0.3 ± 0.008	1.2 ± 0.6	1.1 ± 0.5	7.4 ± 0.4	1.1 ± 0.4	0.6 ± 0.9	1.1 ± 0.6
313.15	0.3 ± 0.5	1.3 ± 0.9	1.2 ± 0.5	7.9 ± 0.6	1.3 ± 0.4	0.8 ± 0.1	1.2 ± 0.9
318.15	0.4 ± 0.1	1.5 ± 0.5	1.4 ± 0.2	8.8 ± 0.6	1.4 ± 0.6	0.9 ± 0.1	1.3 ± 0.8
323.15	0.4 ± 0.6	1.6 ± 0.2	1.4 ± 0.9	9.5 ± 0.3	1.5 ± 0.9	1.0 ± 0.1	1.4 ± 0.6
328.15	0.5 ± 0.1	1.8 ± 0.01	1.5 ± 0.8	10.9 ± 0.001	1.6 ± 0.6	1.1 ± 0.07	1.5 ± 0.9
AH-4							
298.15	0.8 ± 0.5	0.4 ± 0.1	1.3 ± 0.2	3.3 ± 0.5	1.3 ± 0.1	1.2 ± 0.6	0.9 ± 0.01
303.15	0.9 ± 0.7	0.4 ± 0.6	1.4 ± 0.5	4.3 ± 0.2	1.3 ± 0.8	1.4 ± 0.6	1.0 ± 0.3
308.15	1.0 ± 0.6	0.5 ± 0.1	1.5 ± 0.4	5.0 ± 0.2	1.4 ± 0.7	1.5 ± 0.9	1.1 ± 0.3
313.15	1.1 ± 0.5	0.5 ± 0.7	1.6 ± 0.9	5.7 ± 0.1	1.5 ± 0.5	1.7 ± 0.4	1.2 ± 0.4
318.15	1.2 ± 0.6	0.6 ± 0.4	1.8 ± 0.5	6.5 ± 0.1	1.6 ± 0.2	1.8 ± 0.4	1.3 ± 0.6
323.15	1.3 ± 0.6	0.7 ± 0.2	1.9 ± 0.8	7.0 ± 0.8	1.6 ± 0.8	1.9 ± 0.5	1.4 ± 0.9
328.15	1.5 ± 0.8	0.7 ± 0.7	2.1 ± 0.5	7.8 ± 0.7	1.7 ± 0.4	2.0 ± 0.6	1.6 ± 0.1
AH-5							
298.15	1.7 ± 0.4	1.6 ± 0.5	1.8 ± 0.7	9.6 ± 0.1	1.6 ± 0.4	1.9 ± 0.9	1.8 ± 0.7
303.15	1.7 ± 0.6	1.6 ± 0.7	1.9 ± 0.005	9.7 ± 0.2	1.6 ± 0.6	2.0 ± 0.3	1.9 ± 0.9
308.15	1.7 ± 0.9	1.6 ± 0.9	1.9 ± 0.3	9.8 ± 0.2	1.6 ± 0.8	2.0 ± 0.8	2.1 ± 0.2
313.15	1.8 ± 0.3	1.7 ± 0.2	1.9 ± 0.6	10.0 ± 0.1	1.7 ± 0.1	2.1 ± 0.3	2.1 ± 0.9
318.15	1.8 ± 0.5	1.7 ± 0.5	2.0 ± 0.01	10.0 ± 0.1	1.7 ± 0.3	2.1 ± 0.8	2.3 ± 0.2
323.15	1.8 ± 0.8	1.7 ± 0.7	2.0 ± 0.5	10.0 ± 0.4	1.7 ± 0.5	2.2 ± 0.3	2.3 ± 0.8
328.15	1.9 ± 0.2	1.7 ± 0.9	2.0 ± 0.9	10.1 ± 0.7	1.7 ± 0.8	2.2 ± 0.7	2.4 ± 0.8
AH-6							
298.15	0.4 ± 0.6	0.6 ± 0.3	1.4 ± 0.4	7.0 ± 0.6	0.5 ± 0.6	0.6 ± 0.4	0.0 ± 0.7
303.15	0.5 ± 0.7	0.7 ± 0.4	1.5 ± 0.3	7.8 ± 0.5	0.6 ± 0.3	0.7 ± 0.8	0.0 ± 0.7
308.15	0.6 ± 0.4	0.8 ± 0.4	1.6 ± 0.3	8.7 ± 0.3	0.6 ± 0.9	0.8 ± 0.7	0.0 ± 0.7
313.15	0.7 ± 0.1	0.9 ± 0.2	1.7 ± 0.6	9.9 ± 0.4	0.7 ± 0.8	0.9 ± 0.6	0.0 ± 0.7
318.15	0.7 ± 0.9	1.0 ± 0.2	1.8 ± 0.9	10.6 ± 0.5	0.8 ± 0.9	1.0 ± 0.7	0.0 ± 0.7
323.15	0.8 ± 0.8	1.1 ± 0.2	2.0 ± 0.3	11.6 ± 0.3	1.0 ± 0.08	1.1 ± 0.5	0.0 ± 0.7
328.15	0.9 ± 0.7	1.2 ± 0.3	2.1 ± 0.9	12.7 ± 0.6	1.1 ± 0.08	1.2 ± 0.4	0.0 ± 0.7
AH-7							
298.15	2.0 ± 0.9	1.9 ± 0.9	5.4 ± 0.3	15.6 ± 0.3	2.0 ± 0.7	1.9 ± 0.6	0.6 ± 0.6
303.15	2.1 ± 0.4	2.1 ± 0.07	5.5 ± 0.3	15.9 ± 0.2	2.1 ± 0.5	2.0 ± 0.02	0.7 ± 0.9
308.15	2.2 ± 0.3	2.1 ± 0.8	5.6 ± 0.4	16.2 ± 0.2	2.2 ± 0.3	2.0 ± 0.5	0.8 ± 0.9
313.15	2.3 ± 0.0	2.2 ± 0.9	5.7 ± 0.9	16.6 ± 0.6	2.3 ± 0.02	2.1 ± 0.03	0.9 ± 0.9
318.15	2.3 ± 0.9	2.3 ± 0.8	5.9 ± 0.3	17.0 ± 0.5	2.3 ± 0.7	2.1 ± 0.5	1.1 ± 0.09
323.15	2.4 ± 0.4	2.4 ± 0.4	6.0 ± 0.8	17.4 ± 0.8	2.4 ± 0.5	2.2 ± 0.03	1.1 ± 0.8
328.15	2.5 ± 0.4	2.5 ± 0.7	6.1 ± 0.6	17.7 ± 0.3	2.5 ± 0.2	2.2 ± 0.6	1.2 ± 0.9
AH-8							
298.15	0.8 ± 0.3	0.6 ± 0.7	0.6 ± 0.6	4.3 ± 0.4	0.8 ± 0.5	0.7 ± 0.2	0.5 ± 0.9
303.15	0.9 ± 0.8	0.7 ± 0.4	0.7 ± 0.6	5.0 ± 0.3	0.9 ± 0.7	0.8 ± 0.06	0.6 ± 0.8
308.15	1.0 ± 0.9	0.8 ± 0.2	0.8 ± 0.9	5.9 ± 0.3	1.0 ± 0.8	0.9 ± 0.03	0.7 ± 0.9
313.15	1.1 ± 0.6	0.9 ± 0.6	0.9 ± 0.5	6.8 ± 0.8	1.2 ± 0.3	1.0 ± 0.1	0.8 ± 0.6
318.15	1.2 ± 0.8	1.0 ± 0.6	1.0 ± 0.9	7.6 ± 0.07	1.3 ± 0.1	1.1 ± 0.1	0.9 ± 0.8
323.15	1.4 ± 0.3	1.1 ± 0.4	1.1 ± 0.9	8.5 ± 0.8	1.4 ± 0.6	1.2 ± 0.4	1.1 ± 0.03
328.15	1.5 ± 0.7	1.3 ± 0.1	1.3 ± 0.02	9.3 ± 0.9	1.5 ± 0.7	1.3 ± 0.9	1.1 ± 0.8

3.3. Excess enthalpy of solutions

The excess enthalpy (H^E) of solution can provide a more detail information on understanding the behaviour of a solution. This excess enthalpy (H^E) of solution can be evaluated by experimental solubility data and λ parameter of Buchowski-Ksiazczak λ*h* model using the following equation [32]:

$$hR = \Delta_{fus}H + {}^{H^E}\Big/_{x^{exp}} \tag{14}$$

where $\Delta_{fus}H$ is the fusion of enthalpy of compounds, x_{exp} is the solubility data in mole fraction of in solvents and *R* is gas constant. *h* refers the parameter in the Buchowski-Ksiazczak λ*h* model.

The calculated H^E values for all the compounds are listed in Table 9 for the studied solvents in different temperatures. It is observed that table that H^E is positive which increases with increase in temperature. This may be due to contribution of several interactions in the solution. The cavity formation at compounds dissolution requires the absorption of heat to overcome the interactions between the solvents. The intermolecular interactions between compound and solvent molecules are again proved by the positive enthalpy. Therefore, the dissolution of studied compounds needs to absorb energy, so dissolution of compounds is endothermic [33].

4. Conclusions

The solubility of studied compounds is found to increases with increase in temperature. The agreement between experimental solubility data with those evaluated by modified Apelblat and Buchowski–Ksiazczak models is satisfactory. The positive enthalpy and Gibb's free energy of dissolution suggest endothermic and spontaneous dissolution of compounds in all the studied solvents respectively. In all the solvents except 1-butanol, entropy values are found to be negative for the studied compounds, suggesting thereby more ordered structure in solutions.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.molliq.2018.12.081.

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