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SYNTHESIS AND THERMODYNAMIC PROPERTIES OF SOLUTIONS 3-(5-ARYL-2-FURYL) PROPANOIC ACIDS IN ETHYL ACETATE

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Derivatives of 3-(5-aryl-2-furyl)propanoic acids were synthesised for which the process of dissolution in ethyl acetate was studied for the first time. The temperature dependence of solubility was determined experimentally. Based on the results obtained, the enthalpies ($\Delta_{sol}H$) and entropies ($\Delta_{sol}S$) of dissolution were determined. The enthalpy and entropy of fusion of these compounds were calculated using the method of differential thermal analysis. The thermodynamic parameters of melting were recalculated to the standard temperature of 298 K. Using these data, the enthalpy and entropy of mixing in ethyl acetate at 298 K were calculated.

Keywords: enthalpy of dissolution, enthalpy of mixing, enthalpy of fusion, entropy of dissolution, entropy of mixing, entropy of fusion, ethyl acetate, 3-(5-aryl-2-furyl)propanoic acids.

Introduction

Today, the main goal of medicinal chemistry is to develop effective and low-toxic drugs. The search for such drugs is focused mainly on various classes of compounds, especially heterocyclics. Compounds based on the structure of a 5-membered heterocycle with one oxygen atom are widespread in many natural [1–5] and synthetic biologically active substances [6–7], and are also a component of many drugs with various effects (Amiodarone, Cicerfuran, Ailanthoidol, Diloxanide, Mirfentanil, Nitrofurazone, Remdesivir). Recently, furan scaffolds and their functionalised derivatives have been increasingly used in the design of drugs with antimicrobial, anticancer and antiarrhythmic properties [8–10].

The study of the processes of dissolution, synthesis and biological activity of furancarboxylic acid derivatives is an important and relevant scientific task of our time. Therefore, a number of substances that are derivatives of furanpropanoic acids were selected for the study and analysis of the thermodynamic characteristics of solubility.

The aim of this work is to synthesise and experimentally determine the temperature dependence of solubility and calculate the thermodynamic parameters of the process of dissolution of 3-(5-aryl-2-furyl)propanoic acids in ethyl acetate.

Materials and research methods

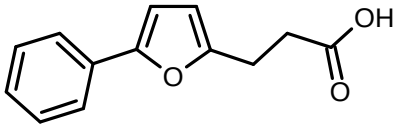
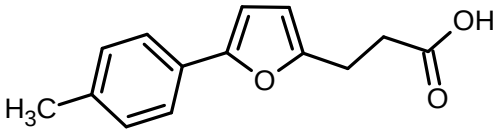
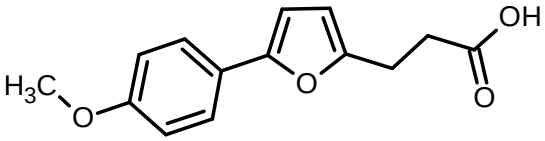
For the study of solubility in ethyl acetate, 3-(5-aryl-2-furyl)propanoic acids were chosen, the structural formulas and some characteristics of which are given in Table 1.

The synthesis of 3-(5-aryl-2-furyl)propanoic acids was carried out by the interaction of 4,7-dioxo-7-phenylheptanoic acids with phosphorus pentoxide, namely, 15 g of phosphorus pentoxide was added to a mixture of 0.1 mol of the corresponding phenacyllevulinic acid and 300 ml of benzene. The mixture was boiled for 2 hours. After cooling, a precipitate was formed, which was filtered off, washed with benzene and hexane and recrystallised from a 2:1 mixture of benzene:hexane.

The structures of compounds I-III were confirmed by IR spectroscopy and elemental analysis.

Table 1

Structural formulas of the substances under study

№	Structural formula	Molecular formula	Molecular mass g/mol
I	***3-(5-phenyl-2-furyl)propanoic acid***		
		$C_{13}H_{12}O_3$	216.23
II	***3-[5-(4-methylphenyl)-2-furyl]propanoic acid***		
		$C_{14}H_{14}O_3$	230.26
III	***3-[5-(4-methoxyphenyl)-2-furyl]propanoic acid***		
		$C_{14}H_{14}O_4$	246.26

3-(5-Phenyl-2-furyl)propanoic acid I. 80 % yield, m.p. 116–117 °C, IR spectrum (ATR, cm-1): 3026.42, 2918.03, 2863.83, 2724.06, 2609.97, 1690.06, 1611.62, 1593.08, 1548.87, 1483.26, 1444.75, 1413.38, 1346.34, 1310.69, 1272.18, 1233. 67, 1210.85, 1178.05, 1072.51, 1056.82, 1019.74, 976.95, 907.07, 847.17, 792.97, 753.04, 686.01, 660.34, 648.93, 527.70, 512.01, 492.04, 459.24. Found, %: C 72.21; H 5.59. C13H12O3. Calculated, %: C 71.78; H 5.14.

3-[5-(4-Methylphenyl)-2-furyl]propanoic acid II. 75 % yield, m.p. 120–121 °C, IR spectrum (ATR, cm-1): 3024.99, 2902.34, 2852.42, 2638.49, 2524.39, 1685.78, 1601.64, 1553.14, 1497.52, 1437.62, 1410.52, 1344.92, 1313.54, 1285.02, 1272.18, 1235.10, 1212.28, 1173.77, 1108.17, 1052.54, 1024.02, 972.68, 949.86, 934.17, 919.91, 817.22, 794.40, 740.20, 658.91, 530.55, 503.45, 470.65. Found, %: C 69.71; H 5.87. C14H14O3. Calculated, %: C 70.03; H 6.13.

3-[5-(4-methoxyphenyl)-2-furyl]propanoic acid III. 70 % yield, m.p. 142–143 °C, IR spectrum (ATR, cm-1): 2916.60, 2835.31, 2641.34, 1690.06, 1617.32, 1598.78, 1578.82, 1553.14, 1498.95, 1437.62, 1419.08, 1344.92, 1304.98, 1289.30, 1235.10, 1170.92, 1109.59, 1025.45, 978.38, 845.74, 830.06, 822.92, 788.70, 654.63, 633.24, 608.99, 526.27, 490.62, 450.68. Found, %: C 68.28; H 5.73. C14H14O4. Calculated, %: C 67.91; H 5.24.

For the study, samples of substances obtained after 3 and 4 times recrystallisation (sample 1 and 2, respectively) were used. The purity of the substances was indirectly confirmed by the stable values of the melting point and the enthalpy of fusion of the samples obtained after different degrees of recrystallisation.

For the solubility studies of 3-(5-phenyl-2-furyl) propanoic acid and its derivatives, ethyl acetate produced by Merck, CAS 71-43-2, with a mass fraction of the basic substance $\geq$ 99.8 % was chosen. Ethyl acetate belongs to the so-called 'high-capacity solvents' and is widely used in the production of coatings, adhesives, pharmaceuticals, and as an extractant in the food industry. Under normal conditions, it is a colourless liquid with a pleasant, fruity odour.

The dissolution process of 3-(5-aryl-2-furyl)propanoic acids was carried out in a sealed vessel with a thermometer, stirrer and a sampling hole. The dissolution vessel was placed in a thermostat that maintained a temperature accuracy of ±0.1 K. Stirring was performed at 30 rpm, and the dissolution process lasted 120 minutes with constant stirring and 60 minutes without stirring. Samples for

analysis were taken after the solution had completely settled. The study was carried out both at increasing and decreasing temperatures. Samples of solutions weighing 1.0–2.0 g were taken and placed in pre-prepared and weighed bureks, which were hermetically sealed and weighed to determine the mass of the saturated solution. After that, the bureaux were opened and the solvent was evaporated in a drying oven at 360 K until a constant weight was reached. The mass of the dry residue was determined by weighing the bullion after drying. Weighing at all stages was carried out on a balance VLR-200 with an accuracy of ±0.0002 g.

Table 2 shows the initial results of the process of dissolution of the test substances in ethyl acetate where the masses of solvent m_1 and solute m_2, g, solubility expressed in mole fractions (x_2) and temperature T, K at which the solubility was determined.

Results and discussion

The experimental data were processed by the least squares method and represented in the linear form of the Schröder equation (1) [11], which is also shown in Table 2.

$$\ln x_2 = -\Delta_{sol}H/RT + \Delta_{sol}S/R, \quad (1)$$

where Δ_{sol}H and Δ_{sol}S are the differential changes in enthalpy and solubility entropy. Hereinafter, the errors of all values are given for a significance level of 0.95.

Table 2

Temperature dependence of the solubility of 3-(5-aryl-2-furyl)propanoic acids

T, K	m_1, g	m_2, g	$x_2 \cdot 10^2$	T, K	m_1, g	m_2, g	$x_2 \cdot 10^2$
1	2	3	4	5	6	7	8
3-(5-phenyl-2-furyl)propanoic acid							
274.4	1.6111	0.1188	2.92	288.2	1.4987	0.1716	4.46
274.4	1.8098	0.1334	2.92	290.0	1.5556	0.1931	4.82
274.4	2.3704	0.1765	2.95	290.0	1.6110	0.1997	4.81
278.0	1.6179	0.1360	3.31	290.0	1.3318	0.1651	4.81
278.0	1.7038	0.1421	3.29	290.5	1.8551	0.2317	4.84
278.0	2.0337	0.1699	3.29	290.5	1.5140	0.1893	4.84
280.2	1.6845	0.1520	3.55	290.5	1.3243	0.1656	4.84
280.2	1.7898	0.1614	3.55	291.5	1.5683	0.2037	5.03
280.2	1.9017	0.1706	3.53	291.5	1.7270	0.2249	5.04
281.5	1.6183	0.1512	3.67	291.5	1.4651	0.1904	5.03
281.5	1.7090	0.1605	3.69	292.8	1.6604	0.2264	5.26
281.5	1.8830	0.1766	3.68	292.8	1.7258	0.2328	5.21
282.2	1.6444	0.1577	3.76	292.8	1.3362	0.1800	5.20
282.2	1.5494	0.1477	3.74	296.8	1.4290	0.2126	5.72
282.2	1.4994	0.1436	3.76	296.8	1.5931	0.2370	5.72
288.2	2.2276	0.2564	4.48	296.8	1.5730	0.2344	5.72
288.2	1.553	0.1774	4.45	**$\ln x_2 = (5.52 \pm 0.13) - (2483 \pm 36) \times 1/T$**			
3-[5-(4-methylphenyl)-2-furyl]propanoic acid							
286.8	2.9804	0.2493	3.10	298.4	1.3566	0.1725	4.64
286.8	2.3624	0.1982	3.11	298.4	1.4596	0.1853	4.63
286.8	2.4520	0.2059	3.11	298.4	1.5998	0.2033	4.64
288.5	3.3846	0.3019	3.30	299.5	1.6997	0.2234	4.79
288.5	3.2397	0.2885	3.30	299.5	1.3025	0.1712	4.79
288.5	2.2039	0.1963	3.30	299.5	0.9441	0.1244	4.80
290.7	1.9500	0.1893	3.58	300.5	1.1001	0.1530	5.05
290.7	2.3801	0.2300	3.57	300.5	2.4651	0.3438	5.07
290.7	2.1008	0.2018	3.55	300.5	2.0265	0.2835	5.08
293.9	1.3680	0.1511	4.05	301.0	1.3066	0.1844	5.12
293.9	1.2773	0.1408	4.04	301.0	1.3111	0.1852	5.13
293.9	1.3753	0.1517	4.05	303.1	1.3088	0.1957	5.41

Continuation Table 2

1	2	3	4	5	6	7	8
296.5	1.2783	0.1534	4.39	303.1	1.2918	0.1933	5.42
296.5	1.4400	0.1737	4.41	303.1	1.2521	0.1881	5.44
296.5	1.4038	0.1681	4.38	305.0	1.3151	0.2146	5.88
297.8	1.3518	0.1700	4.59	305.0	1.2557	0.2045	5.86
297.8	1.2192	0.1533	4.59	305.0	1.6067	0.2620	5.87
297.8	1.5505	0.1951	4.59	**$\ln x_2 = (7.08\pm0.13) - (3029\pm40) \times 1/T$**			
3-[5-(4-methoxyphenyl)-2-furyl]propanoic acid							
277.6	1.2355	0.0287	0.82	289.9	1.1469	0.03685	1.14
277.6	1.5042	0.0347	0.82	289.9	1.5482	0.0497	1.14
277.6	1.7056	0.0396	0.82	289.9	1.72735	0.05535	1.13
281.2	1.2552	0.0318	0.90	291.6	0.9981	0.03365	1.19
281.2	1.2996	0.0332	0.91	291.6	1.76285	0.05975	1.20
281.2	1.5332	0.0392	0.91	291.6	1.96415	0.0664	1.20
285.4	1.0742	0.0313	1.03	293.8	1.272	0.04545	1.26
285.4	1.5741	0.0456	1.03	293.8	1.3649	0.0488	1.26
285.4	1.2850	0.0371	1.02	293.8	1.24475	0.0445	1.26
287.9	1.2982	0.0398	1.09	295.9	1.1968	0.0454	1.34
287.9	1.5937	0.0494	1.10	295.9	1.27545	0.0482	1.33
287.9	1.3936	0.0429	1.09	295.9	1.32535	0.0499	1.33
$\ln x_2 = (2.99\pm0.12) - (2162\pm34) \times 1/T$							

Differential changes in the enthalpy ($\Delta_{sol}H^o$) and entropy ($\Delta_{sol}S^o$) of dissolution of the substances studied in this work were calculated using the temperature dependence of solubility (Table 2) according to Equations 2–3. which include the mixing processes ($\Delta_{mix}H^o$; $\Delta_{mix}S^o$) and the phase transition of the crystalline substance into the liquid phase of the solution ($D_{fus}H^o$; $D_{fus}S^o$). (equations 4–5) are given in Table 3.

$$\Delta_{sol}H^o = R \cdot B, \quad (2)$$

$$\Delta_{sol}S^o = R \cdot A, \quad (3)$$

$$\Delta_{sol}H^o = \Delta_{mix}H^o + \Delta_{fus}H, \quad (4)$$

$$\Delta_{sol}S^o = \Delta_{mix}S^o + \Delta_{fus}S^o \quad (5)$$

Table 3

Thermodynamic parameters of solubility of 3-(5-aryl-2-furyl)propanoic acids in ethyl acetate at 298 K

Substance	$x_2 \cdot 10^3$	$\Delta_{sol}H^o$	$\Delta_{mix}H^o$	$\Delta_{sol}S^o$	$\Delta_{mix}S^o$
		kJ/mol		J/ mol›K	
I	60.1	20.64±0.30	-3.3±2.0	45.9±1.1	-13.5±3.6
II	46.2	25.18±0.32	-3.7±1.8	58.9±1.2	-11.9±4.7
III	14.1	17.97±0.29	-14.9±2.2	24.8±1.0	-50.5±3.6

The melting enthalpies ($\Delta_{fus}H$) of the studied substances were determined by differential thermal analysis using a Paulik-Paulik-Erdey Q-1500 D derivatograph. The samples were analysed in a dynamic mode at a heating rate of 5K/min in an air atmosphere.

To calculate $\Delta_{fus}H$. we used the thermochemical equation (6). which takes into account the correction for the possible mass loss of the sample during the melting process:

$$K \cdot S = q_{fus} + q_{vap} = m_o \cdot \Delta_{fus}H + \Delta m_{vap} \cdot \Delta_{vap}H, \quad (6)$$

where q_{fus} and q_{vap} is the amount of heat (J) absorbed during the melting and evaporation of the sample. respectively; mo is the mass of the sample (g) corresponding to the temperature of its melting point T_{fus}; Dm_{vap} is the mass loss of the sample (vapour mass. g) over the period taken into account to determine the peak area S (K·s) under the DTA curve; K is the heat transfer coefficient of the derivatograph K = 8.202-10-5· T*fus* (J/K·s); D_{fus}H and D_{vap}H are the specific enthalpies of melting and evaporation of the substance (J/g).

Table 4 shows the results of determining the thermodynamic parameters of the melting process at their melting point (T_{fus})

Table 4

Thermodynamic parameters of the melting process of 3-(5-aryl-2-furyl)propanoic acids

The number	m_0, g	$\Delta m_{vap}\cdot 10^3$, g	S, K·s	q_{vap}, J	$\Delta_{fus}H_{Tfus}$, kJ/mol	$\Delta_{fus}S_{Tfus}$, J/mol
3-(5-phenyl-2-furyl)propanoic acid T_{fus}= 390.5±1.5 K; K = 0.03203 J/K·s						
1	0.1020	0.286	423.2	0.1113	28.5	73.0
1	0.1005	0.151	430.8	0.0588	29.6	75.8
2	0.1145	0.650	486.0	0.2548	28.9	74.0
Average values:					29.0± 1.3	74.3± 3.5
3-[5-(4-methylphenyl)-2-furyl]propanoic acid T_{fus}= 394.4±1.5K; K = 0.03235 J/K·s						
1	0.1024	0.281	504.7	0.1089	36.47	92.5
1	0.1105	0.360	515.8	0.1394	34.48	87.4
2	0.1209	0.580	571.8	0.2246	34.81	88.3
Average values:					35.3± 1.6	89.4± 6.7
3-[5-(4-methoxyphenyl)-2-furyl]propanoic acid T_{fus}= 416.5±1.1K; K = 0.03416 J/K·s						
1	0.1018	0.400	509.6	0.1330	41.8	100.4
1	0.1099	0.492	540.2	0.1635	41.0	98.4
2	0.1058	0.385	536.2	0.1280	42.3	101.6
Average values:					41.7± 1.5	100.1± 4.0

The change in entropy at the melting point ($\Delta_{fus}S_{Tfus}$) was calculated using Equation (7). The results are shown in Table 4.

$$\Delta_{fus}S_{T_{fus}} = \Delta_{fus}H_{T_{fus}} / T_{fus} . \qquad (7)$$

The thermodynamic parameters determined during the experimental studies belong to different temperatures. for example. $\Delta_{sol}H^o$ and $\Delta_{sol}S^o$ were calculated in the temperature range given in Table 2. and the value of $\Delta_{fus}H^o$ was determined at the melting point of the substance. To summarise the results and calculate the thermodynamic parameters ($\Delta_{mix}H^o$; $\Delta_{mix}S^o$) at the generally accepted temperature of 298 K. it became necessary to recalculate the values of $\Delta_{fus}H^o$; $\Delta_{fus}S^o$ to 298 K. For this conversion, we used Equations 8 and 9, which were obtained as a result of analytical processing of an array of experimentally determined values of enthalpy, entropy, and heat capacity changes during the melting process.

$$\Delta_{fus}H_T = \Delta_{fus}H_{T_{fus}}\left[1 + \frac{T-T_{fus}}{1.35\cdot T_{fus}}\right], \qquad (8)$$

$$\Delta_{fus}S_T = \Delta_{fus}S_{T_{fus}}\left[1 + 0.74\cdot ln\frac{T}{T_{fus}}\right]. \qquad (9)$$

The following values were calculated by recalculating the entropy and enthalpy of fusion to 298 K: - 3-(5-phenyl-2-furyl)proacetic acid; $\Delta_{fus}H_{298}$ = = 23.9±2.1 kJ/mol, $\Delta_{fus}S_{T_{298}}$ = 59.4±3.4 J/(mol·K); -3-[5-(4-methylphenyl)-2-furyl]propanoic acid; $\Delta_{fus}H_{298}$ = 28.9±2.3 kJ/mol, $\Delta_{fus}S_{T_{298}}$ = 70.9± ±3.7 J/mol·K; -3-[5-(4-methoxyphenyl)-2-furyl] propanoic acid; $\Delta_{fus}H_{298}$ = 32.9±2.2 kJ/mol, $\Delta_{fus}S_{T_{298}}$ = =75.3±3.5 J/mol·K.

Using the calculated values of the thermodynamic parameters of the melting process according to Equations 4 and 5, we determined $\Delta_{mix}H$ and $\Delta_{mix}S^o$, the values of which are given in Table 3.

Judging from the results of calculating $\Delta_{mix}H$ and $\Delta_{mix}S^o$ of the substances studied in this work with ethyl acetate. it can be concluded that the interactions that occur between the solvent and the dissolved substances are of the same type, as evidenced by the presence of the so-called compensatory effect not only for the solutions studied in this work, but also for other solutions formed with the participation of aryl furan acids with ethyl acetate (see Fig.). For the joint analysis, a number of compounds were chosen that are structurally related to arylfuran acids, and their thermodynamic properties of solutions were studied in ethyl acetate [12].

Regarding the values of the thermodynamic parameters of the mixing process of the compounds studied in this work, the negative values of $\Delta_{mix}H^o$ ((-3.3±2.0) and (-3.7±1.8) kJ/mol) indicate the formation of somewhat stronger intermolecular interactions between the components after mixing.

The joint dependence of the enthalpy change on the entropy of mixing of the substances (I-III) studied in this work and the thermodynamic parameters of the process of mixing arylfuran derivatives in ethyl acetate. the values of which are given in Table 5. $\Delta_{mix}H_{298} = 0.351161 \times \Delta_{mix}S_{298} + 2.13201$; $R^2 = 0.9196$

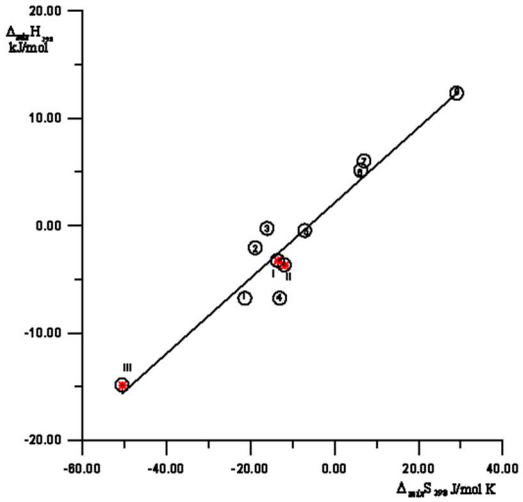


Table 5

Thermodynamic parameters of the process of mixing aryl furan derivatives in ethyl acetate

The number of the point on the graph	Name of the compound	$\Delta_{mix}H_{298}$. kJ/mol	$\Delta_{mix}S_{298}$. J/mol·K
1	2-methyl-5-phenylfuran-3-carboxylic acid	-6.8±1.9	-21.3±4.3
2	2-methyl-5-(4-methylphenyl)-furan-3-carboxylic acid	-2.1±1.6	-18.8±4.2
3	3-[5-(2-nitrophenyl)-2-furyl] acrylic acid	-0.3±1.4	-16.0±3.8
4	2-methyl-5-(2-chloro-5-trifluoromethylphenyl)-furan-3-carboxylic acid	-6.8±5.1	-13±10
5	2-methyl-5-(2.5-dichlorophenyl)-furan-3-carboxylic acid	-0.5±4.9	-7.0±9.1
6	5-(3-nitrophenyl)-furan-2-carboxylic acid	5.1±4.1	6.3±8.0
7	5-(2-nitrophenyl)-furan-2-carboxylic acid	6.0±1.5	7.1±3.6
8	5-(4-nitrophenyl)-furan-2-carboxylic acid	12.3±4.1	29.1±8.1

Regarding the values of the thermodynamic parameters of the mixing process of the compounds studied in this work, the negative values of $\Delta_{mix}H^o$ ((-3.3 ± 2.0) and (-3.7 ± 1.8) kJ/mol) indicate the formation of somewhat stronger intermolecular interactions between the components after mixing.

Such values will be typical for substances with similar polarity or for molecules that do not form strong specific interactions (hydrogen bonds. ionic interactions. etc.). For the compound with an oxymethyl group (III), the value is slightly different from the previous $\Delta_{mix}H^o$ ((-14.9 ± 2.2) kJ/mol) due to the formation of stronger interactions due to the methoxy group, whose elements can form hydrogen bonds, ion-dipole interactions. or associations with ethyl acetate.

Conclusions

Based on the results of experimental studies, the solubility of 3-(5-phenyl-2-furyl)propanoic acid; 5-(4- methylphenyl-2-furyl)propanoic acid; 3-[5-(4-methoxyphenyl)-2-furyl]propanoic acid was synthesised and the temperature dependences of its solubility were determined for the first time. The thermodynamic parameters of the dissolution process were calculated. The presence of a compensatory effect was established, which confirms the homogeneity of the interaction of dissolved substances with ethyl acetate. The energies of intermolecular interactions in the studied arylfuranic acids were analysed.

The experimentally determined and calculated thermodynamic parameters of the dissolution process will be used in the development (optimisation) of technological processes for the synthesis, purification or processing of the substances studied in this work, and can also be used to predict the thermodynamic parameters of the dissolution process of newly synthesised aryl furan derivatives with a carboxyl group.

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СИНТЕЗ ТА ТЕРМОДИНАМІЧНІ ВЛАСТИВОСТІ РОЗЧИНІВ 3-(5-АРИЛ-2-ФУРИЛ)ПРОПАНОВИХ КИСЛОТ У ЕТИЛАЦЕТАТІ

Синтезовано та вперше досліджено процес розчинення похідних 3-(5-арил-2-фурил) пропанових кислот у етилацетаті. Встановлено температурні залежності розчинності експериментальним шляхом. На основі отриманих результатів визначено ентальпії ($\Delta_{sol}H$) та ентропії ($\Delta_{sol}S$) розчинення. Методом диференційно-термічного аналізу розраховано ентальпію та ентропію плавлення цих сполук. Термодинамічні параметри плавлення приведено до стандартної температури 298 К. На їх основі проведено розрахунок ентальпії та ентропії змішування у етилацетаті за 298 К.

Ключові слова: ентальпія розчинення, ентальпія змішування, ентальпія плавлення, ентропія розчинення, ентропія змішування, ентропія плавлення, етилацетат, 3-(5-арил-2-фурил)пропанові кислоти.