

АНАЛІТИЧНА ХІМІЯ. ФІЗИЧНА ТА КОЛОЇДНА ХІМІЯ.  
НЕОРГАНІЧНА ХІМІЯ. ОРГАНІЧНА ХІМІЯ

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SOLUBILITY OF 5-(4-METHYLPHENYL)-2-FURANPROPANOIC ACID  
IN SOME ORGANIC SOLVENTS

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**In this study, the temperature dependences of the solubility of 5-(4-methylphenyl)-2-furanpropanoic acid in various solvents were evaluated: methyl and ethyl acetate, acetonitrile, propan-1-ol, and propan-2-ol. The results of the analysis are presented in the form of linear equations according to the Schröder model, which allowed us to determine the enthalpies, entropies, and Gibbs energies of solubility at a temperature of 298.15 K. The melting points of the acid were determined using the method of differential thermal analysis, which allowed us to calculate the enthalpies, entropies, and Gibbs energies of mixing.**

**Key words: solubility; enthalpy of dissolution; enthalpy of mixing; enthalpy of fusion; 5-(4-methylphenyl)-2-furanpropanoic acid.**

### Introduction

Furan derivatives are important in medicinal chemistry because of their unique role. Incorporating the furan ring into drug synthesis is an important strategy in drug development. The high therapeutic properties of furan drugs encourage chemists to synthesize a large number of new chemotherapeutic agents [1–3]. It should be emphasized that furans and tetrahydrofurans are well-known drugs that are actively used in medicine and veterinary medicine, such as Nitrofurantoin, Nitrofurantoin, Lazalocid (antibacterial agents); Nifurtimox (antiparasitic drug); Naftidrofuryl (peripheral vasodilator); Ranitidine (H<sub>2</sub> histamine antagonist); as well as Ribavirin, Taribavirin, Remdesivir and Molnupiravir (drugs for the treatment of viral infections, including COVID-19) [4–7]. Thus, the further development of the synthesis of new compounds with the furan ring is an urgent goal not only for organic chemistry, but also for medicine, materials science, and other fields.

In this regard, it is becoming increasingly important to apply the latest unified methods for the

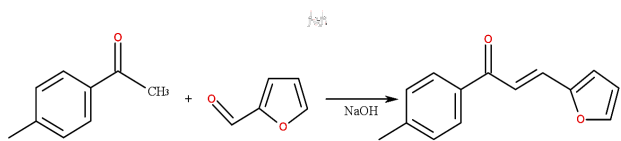
synthesis, purification, and analysis of medicines, both at manufacturing plants and in quality control systems operating at the state level. Despite the wide range of applications of furan derivatives, determining their thermodynamic characteristics is an urgent task. In today's world, thermodynamic research methods remain one of the most reliable and effective ways to analyze metabolism and energy in living systems, reactors, and other technical systems. **The purpose of this study** was to analyze the thermodynamic characteristics of the solubility of 5-(4-methylphenyl)-2-furanpropanoic acid in various organic solvents.

### Materials and research methods

To study the thermodynamic parameters of solubility in methyl- and ethyl acetate, acetonitrile, propan-1-ol, and propan-2-ol, 5-(4-methylphenyl)-2-furanpropanoic acid was chosen.

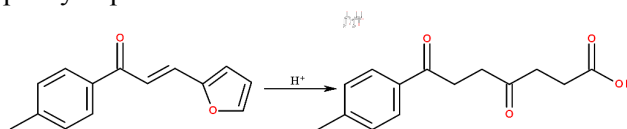
The synthesis of 5-(4-methylphenyl)-2-furanpropanoic acid was carried out in three steps. In the

first step, furfurylidene acetophenone was synthesized.



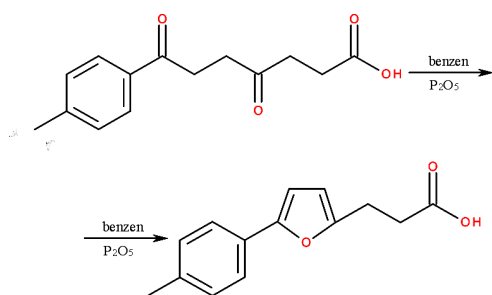
To a mixture of 100 g of acetophenone, 80 g of furfural in 200 ml of methanol with intense stirring, add 0.05 mol of KOH in the form of a 15 % solution. The temperature is maintained in the range of 293–298 K (water bath). The reaction mixture is stirred for 3 hours, neutralized with acetic acid, diluted with 400 mL of water, extracted with methylene chloride, washed with water and separated on a separating funnel, dried with sodium sulfate. The solvent is distilled off, the residue is distilled in vacuum at 423K/2 mm·Hg.

At the second stage 4,7-dioxo-7-4-methylphenylheptanoic acid was obtained.



A mixture of 0.2 mol of the corresponding furfurylideneacetophenone, 300 mL of ethyl alcohol, 90 mL of con. HCl and 15 mL of water were refluxed for 24 h. The alcohol was distilled off under reduced pressure, and 200 mL of brine, 200 mL of ice-cold water were added to the resulting black viscous mass. HCl, 200 mL of ice-cold acetic acid, 400 mL of water were added to the resulting black viscous mass and heated under reflux condenser for 3 h. After cooling, the formed light yellow crystalline precipitate was decanted from the residual resin, filtered, washed three times with cold water and recrystallized from aqueous alcohol. The yield was 65 %, m. p. 386–387 K.

The last step is the direct synthesis of 5-(4-methylphenyl)-2-furanpropanoic acid.



To a mixture of 0.1 mol of 4,7-dioxo-7-4-methylphenylheptanoic acid and 300 mL of benzene

was added 15 g of phosphorus pentoxide. The mixture was boiled for 2 hours. After cooling, a precipitate was formed, which was filtered off, washed with benzene and hexane, and recrystallized from a 2:1 mixture of benzene:hexane. The yield was 75 %. m.p. 393–394 K. Found, %: C 69.71; H 5.87.  $C_{14}H_{14}O_3$ . Calculated, %: C 70.03; H 6.13.

For solubility studies, the substances obtained after 3 and 4-fold recrystallization were used. The purity of the acid was indirectly confirmed by the unchanged values of the melting point and the value of the enthalpy of fusion of the samples taken after different degrees of recrystallization.

To study the solubility of 5-(4-methylphenyl)-2-furanpropanoic acid, a number of widely used organic solvents with a boiling point of up to 371 K and different polarities were chosen, namely acetonitrile  $CH_3CN$  manufactured by Merck; CAS No. 75-05-8; EC No. 200-835-2; mass fraction of the main substance  $\geq 99.9$  % by weight; methyl acetate ( $C_3H_6O_2$ ) manufactured by Merck; CAS No. 79-20-9; EC No. 201-185-2; mass fraction of the main substance  $\geq 99.0$  % by weight; ethyl acetate ( $C_4H_8O_2$ ) manufactured by Merck; CAS No. 71-43-2; EC No. 200-753-7; w/w  $\geq 99.8$  %; propan-1-ol ( $C_3H_8O$ ); CAS No. 71-23-8; EC No. 200-746-9; w/w  $\geq 99.5$  %; propan-2-ol ( $C_3H_8O$ ); CAS No. 67-63-0; EC No. 200-661-7; w/w  $\geq 99.8$  % This work continues the series of our studies on determining the thermodynamic properties of solubility of acids, aldehydes and their derivatives with an aryl furan fragment in a number of organic solvents of different polarity [8–10].

The dissolution of 5-(4-methylphenyl)-2-furanpropanoic acid was carried out in a sealed vessel equipped with a thermometer, stirrer, and a sampling hole. The vessels in which the dissolution was carried out were immersed in a thermostat, the accuracy of thermostatization was  $\pm 0.1$  K. The stirring speed was 30 rpm; the dissolution time was 180 min with constant stirring. Sampling was carried out after its complete precipitation. To confirm the establishment of equilibrium, the experiments were carried out both in the mode of temperature increase and decrease; the absence of a hysteresis loop on the temperature dependence curves of solubility confirms the achievement of a state close to equilibrium. Samples of solutions weighing 0.5–0.7 g were taken and placed in pre-prepared and weighed bureaus, after which they were hermetically

sealed and weighed, thus determining the mass of the saturated solution. Then, the bureaus were opened and placed in a drying oven, where the solvent was evaporated at a temperature of 323–333 K to a constant weight. The mass of the dry residue was determined by weighing the bullion with the substance after drying. Weighing at all stages was carried out on a balance VLR-200 with an accuracy of  $\pm 0.0002$  g.

The enthalpy of vaporization ( $\Delta_{fus}H$ ) of 5-(4-methylphenyl)-2-furanpropanoic acid was determined by differential thermal analysis (DTA). The samples were analyzed on a Paulik-Paulik-Erdey Q-1500 D derivatograph in dynamic mode at a heating rate of 5 K/min in an air atmosphere.

To calculate  $\Delta_{fus}H$ , we used the thermochemical equation (1), which takes into account the correction for the possible mass loss of the sample during the melting process:

$K \cdot S = q_{fus} + q_{vap} = m_o \cdot \Delta_{fus}H + \Delta m_{vap} \cdot \Delta_{vap}H$ , (1)  
where  $q_{fus}$  and  $q_{vap}$  – are the amount of heat (J) absorbed during the melting and vaporization of the sample, respectively;  $m_o$  – is the mass of the sample (g) corresponding to the temperature of its melting onset  $T_{fus}$ ;  $\Delta m_{vap}$  – is the mass loss of the sample

(vapor mass, g) during the period taken into account to determine the peak area  $S$  (K·s) under the DTA curve;  $K$  – is the heat transfer coefficient, J/K·s, for the used installation equal to  $K = 8.202 \cdot 10^{-5}$ ;  $\Delta_{fus}H$ ,  $\Delta_{vap}H$  – are the specific enthalpies of fusion and evaporation of the substance, J/g.

$\Delta_{vap}H$  was calculated from the thermogravimetric analysis according to the method described in [8].

## Results and discussion

Table 1 shows the primary results of the dissolution of 5-(4-methylphenyl)-2-furylpropanoic acid, where the masses of solvent  $m_1$  and solute  $m_2$ , g, are indicated; solubility expressed in mole fractions ( $x_2$ ); temperature  $T$ , K at which the solubility was determined. The experimental data were processed by the least squares method and presented in the linear form of the Schröder equation (2) [11], which is also presented in Table 1

$$\ln x_2 = -\Delta_{sol}H/RT + \Delta_{sol}S/R, \quad (2)$$

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

Table 1

Temperature dependence of solubility of 5-(4-methylphenyl)-2-furanpropanoic acid in organic solvents

$T$ , K	$m_1$ , g	$m_2$ , g	$X_2 \cdot 10^2$	$T$ , K	$m_1$ , g	$m_2$ , g	$X_2 \cdot 10^2$	$T$ , K	$m_1$ , g	$m_2$ , g	$X_2 \cdot 10^2$
1	2	3	4	5	6	7	8	9	10	11	12
<i>methyl acetate</i>											
275.5	1.7362	0.1404	2.54	283.9	1.4204	0.1559	3.41	298.6	1.8604	0.3354	5.48
275.5	1.3031	0.1048	2.52	285.5	1.2157	0.1412	3.60	298.6	1.6164	0.2879	5.41
275.5	1.8763	0.1516	2.53	285.5	1.5040	0.1743	3.59	299.0	1.3527	0.2583	5.79
276.5	1.3310	0.1093	2.57	285.5	1.6924	0.1957	3.59	299.0	1.1416	0.2172	5.77
276.5	1.5033	0.1243	2.59	290.3	0.7548	0.1035	4.22	299.0	1.1786	0.2246	5.78
276.5	1.8228	0.1511	2.60	290.3	1.0052	0.1374	4.21	300.0	1.0963	0.2144	5.92
278.2	1.3008	0.1149	2.76	290.3	1.1361	0.1564	4.24	300.0	1.5402	0.2991	5.88
278.2	1.5131	0.1334	2.76	292.8	0.7161	0.1041	4.47	300.0	1.4366	0.2798	5.90
278.2	1.8452	0.1631	2.76	292.8	0.9248	0.1356	4.50	300.5	1.1765	0.2228	5.74
280.6	1.6488	0.1573	2.98	292.8	0.8250	0.1242	4.62	300.5	1.3513	0.2568	5.76
280.6	1.5432	0.1474	2.98	297.3	1.4082	0.2463	5.33	300.5	1.7297	0.3264	5.72
280.6	1.5854	0.1506	2.97	297.3	1.3574	0.2348	5.27	302.0	0.8372	0.1725	6.22
283.9	1.4170	0.1569	3.44	297.3	1.1264	0.1953	5.28	302.0	1.1606	0.2419	6.28
283.9	1.4072	0.1567	3.46	298.6	1.2813	0.2270	5.39	$\ln x_2 = (6.58 \pm 0.16) - (2830 \pm 45) \times 1/T$			
<i>ethyl acetate</i>											
286.8	2.9804	0.2493	3.10	296.5	1.2783	0.1534	4.39	300.5	1.1001	0.1530	5.05
286.8	2.3624	0.1982	3.11	296.5	1.4400	0.1737	4.41	300.5	2.4651	0.3438	5.07
286.8	2.4520	0.2059	3.11	296.5	1.4038	0.1681	4.38	300.5	2.0265	0.2835	5.08

Continuation of Table 1

1	2	3	4	5	6	7	8	9	10	11	12
288.5	3.3846	0.3019	3.30	297.8	1.3518	0.1700	4.59	301.0	1.3066	0.1844	5.12
288.5	3.2397	0.2885	3.30	297.8	1.2192	0.1533	4.59	301.0	1.3111	0.1852	5.13
288.5	2.2039	0.1963	3.30	297.8	1.5505	0.1951	4.59	303.1	1.3088	0.1957	5.41
290.7	1.9500	0.1893	3.58	298.4	1.3566	0.1725	4.64	303.1	1.2918	0.1933	5.42
290.7	2.3801	0.2300	3.57	298.4	1.4596	0.1853	4.63	303.1	1.2521	0.1881	5.44
290.7	2.1008	0.2018	3.55	298.4	1.5998	0.2033	4.64	305.0	1.3151	0.2146	5.88
293.9	1.3680	0.1511	4.05	299.5	1.6997	0.2234	4.79	305.0	1.2557	0.2045	5.86
293.9	1.2773	0.1408	4.04	299.5	1.3025	0.1712	4.79	305.0	1.6067	0.2620	5.87
293.9	1.3753	0.1517	4.05	299.5	0.9441	0.1244	4.80	ln $x_2=(7.08\pm 0.13)-(3029\pm 40)\times 1/T$			
<i>acetonitrile</i>											
282.0	1.4037	0.0604	0.761	295.8	1.5824	0.1016	1.13	300.0	0.7921	0.0553	1.23
282.0	1.2714	0.0548	0.762	295.8	1.3134	0.0843	1.12	300.0	1.3662	0.0953	1.23
282.0	1.3036	0.0560	0.760	295.8	1.3231	0.0850	1.13	300.0	1.8170	0.1268	1.23
283.6	1.2569	0.0569	0.801	296.7	1.1437	0.0747	1.15	301.4	1.3146	0.0961	1.28
283.6	1.4399	0.0649	0.797	296.7	1.6823	0.1103	1.15	301.4	1.5116	0.1109	1.29
283.6	1.1085	0.0499	0.796	296.7	1.8048	0.1185	1.16	301.4	1.6546	0.1213	1.29
285.3	5.2070	0.2457	0.834	298.2	1.3569	0.0904	1.17	303.8	1.5437	0.1214	1.38
285.3	2.4837	0.1185	0.843	298.2	1.4063	0.0941	1.18	303.8	1.6579	0.1305	1.38
285.3	4.8347	0.2279	0.833	298.2	1.3594	0.0912	1.18	303.8	1.4557	0.1144	1.38
292.5	1.0228	0.0590	1.02	299.0	1.0193	0.0698	1.21	305.5	2.5024	0.2067	1.45
292.5	0.9583	0.0553	1.02	299.0	1.6420	0.1124	1.21	305.5	1.6689	0.1380	1.45
292.5	0.9458	0.0548	1.02	299.0	1.5633	0.1070	1.21	ln $x_2=(3.36\pm 0.12)-(2323\pm 35)\times 1/T$			
<i>propane-1-ol</i>											
279.1	1.2351	0.0652	1.36	284.5	1.3616	0.0914	1.72	292.8	1.2172	0.1191	2.49
279.1	1.4171	0.0747	1.35	285.8	1.2985	0.0930	1.83	295.4	1.3372	0.1399	2.66
279.1	1.3864	0.0730	1.36	285.8	1.3850	0.0989	1.83	295.4	1.5041	0.1596	2.70
280.8	1.3140	0.0741	1.45	287.2	1.1090	0.0826	1.91	295.4	1.1489	0.1219	2.70
280.8	1.5154	0.0849	1.44	287.2	1.1339	0.0838	1.89	296.9	0.9783	0.1104	2.86
280.8	1.7939	0.1012	1.45	287.2	1.4678	0.1108	1.93	296.9	1.6833	0.1972	2.97
282.4	1.6921	0.1009	1.53	289.3	1.3959	0.1154	2.11	296.9	1.6682	0.1895	2.88
282.4	1.2451	0.0748	1.54	289.3	1.4563	0.1210	2.12	299.8	0.9485	0.1230	3.27
282.4	1.1218	0.0670	1.53	289.3	1.2204	0.1016	2.13	299.8	1.0756	0.1402	3.29
284.5	1.2256	0.0818	1.71	292.8	1.4444	0.1412	2.49	299.8	1.0437	0.1359	3.29
284.5	1.4222	0.0956	1.72	292.8	1.5592	0.1540	2.51	ln $x_2=(8.56\pm 0.20)-(3593\pm 57)\times 1/T$			
<i>propane-2-ol</i>											
278.4	1.2241	0.0706	1.48	284.8	1.5290	0.1162	1.94	291.6	1.1525	0.1141	2.52
278.4	1.9475	0.1128	1.49	287.3	1.3249	0.1111	2.14	294.0	1.3088	0.1396	2.71
278.4	1.9030	0.1098	1.48	287.3	1.6325	0.1363	2.13	294.0	1.4522	0.1539	2.69
283.5	1.5006	0.1060	1.81	289.6	1.0688	0.0999	2.38	294.0	1.4699	0.1577	2.72
283.5	1.7093	0.1206	1.80	289.6	1.6756	0.1563	2.38	297.2	1.5295	0.1807	2.99
283.5	1.3635	0.0965	1.81	289.6	1.7559	0.1665	2.41	297.2	1.5248	0.1819	3.02
284.1	1.4915	0.1081	1.86	290.3	1.1521	0.1063	2.35	297.2	1.8808	0.2244	3.02
284.1	1.4378	0.1044	1.86	290.3	1.6071	0.1509	2.39	301.0	1.2674	0.1820	3.61
284.1	1.1350	0.0826	1.86	290.3	1.4480	0.1325	2.33	301.0	1.3514	0.1946	3.62
284.8	1.4677	0.1107	1.93	291.6	1.2535	0.1238	2.51	301.0	1.0794	0.1546	3.60
284.8	1.4943	0.1140	1.95	291.6	1.4481	0.1439	2.52	ln $x_2=(7.37\pm 0.27)-(3226\pm 77)\times 1/T$			

Table 2

**Thermodynamic parameters of solubility of 5-(4-methylphenyl)-2-furanpropanoic acid  
in organic solvents at 298.15K**

No.	Solvent	$x_2 \cdot 10^3$	$\Delta_{sol}H^{\circ}$	$\Delta_{mix}H^{\circ}$	$\Delta_{sol}S^{\circ}$	$\Delta_{mix}S^{\circ}$	$\Delta_{mix}G^{\circ}$
			kJ/mol		J/mol K		kJ/mol K
1	acetonitrile	0.0118	19.3±0.29	-9.6±1.8	27.9±1.0	-42.9±4.6	3.2±1.8
2	methyl acetate	0.0541	23.53±0.37	-5.4±1.8	54.8±1.3	-16.0±4.7	-0.6±1.8
3	ethyl acetate	0.0462	25.18±0.32	-3.7±1.8	58.9±1.2	-11.9±4.7	-0.2±1.8
4	propane-1-ol	0.0303	29.90±0.73	1.0±1.9	71.5±1.7	0.7±4.8	0.8±1.9
5	propan-2-ol	0.0319	26.82±0.64	-2.1±1.9	61.4±2.2	-9.4±5.0	0.7±1.9

Table 3

**Samples enthalpies of fusion of 5-(4-methylphenyl)-2-furanpropanoic acid**

$m_0, g$	$\Delta m_{vap} \cdot 10^3 g$	$S, K \cdot c$	$q_{vap}, Дж$	$\Delta_{fus}H_{T_{fus}},$ kJ/mol	$\Delta_{fus}H_{298.15},$ kJ/mol	$\Delta_{fus}S_{T_{fus}},$ J/mol K	$\Delta_{fus}S_{298.15},$ J/mol K
$T_{fus} = 394.4 \pm 1.5 K; K = 0.03235 J/K \cdot s$							
0.1024	0.281	504.7	0.1089	36.47	29.89	92.5	73.3
0.1105	0.360	515.8	0.1394	34.48	28.23	87.4	69.3
0.1209	0.580	571.8	0.2246	34.81	28.50	88.2	69.9
Mean values:				35.3±1.6	28.9±1.8	89.4±4.1	70.8±4.5

Differential changes in enthalpy ( $\Delta_{sol}H^{\circ}$ ) and entropy ( $\Delta_{sol}S^{\circ}$ ) of acid dissolution were calculated using the temperature dependence of solubility ( $\ln x_2 = A + B/T$ ) (Table 1) according to equations (3)–(4) and are presented in Table 2:

$$\Delta_{sol}H^{\circ} = R \cdot B, \quad (3)$$

$$\Delta_{sol}S^{\circ} = R \cdot A. \quad (4)$$

As known [12] the calculated thermodynamic parameters of dissolution  $\Delta_{sol}H^{\circ}$  i  $\Delta_{sol}S^{\circ}$  include the mixing processes ( $\Delta_{mix}H^{\circ}$ ;  $\Delta_{mix}S^{\circ}$ ) and the phase transition of the crystalline substance into the liquid phase of the solution ( $\Delta_{fus}H^{\circ}$ ;  $\Delta_{fus}S^{\circ}$ ) equations (5), (6):

$$\Delta_{sol}H^{\circ} = \Delta_{mix}H^{\circ} + \Delta_{fus}H^{\circ}, \quad (5)$$

$$\Delta_{sol}S^{\circ} = \Delta_{mix}S^{\circ} + \Delta_{fus}S^{\circ}, \quad (6)$$

The results of determining the enthalpy and entropy of fusion of the studied acids are presented in Table 3.

The change in entropy at the melting temperature ( $\Delta_{fus}S_{T_{fus}}$ ) the values of which are given in the Table 3 was calculated according to equation (7)

$$\Delta_{fus}S_{T_{fus}} = \frac{\Delta_{fus}H_{T_{fus}}}{T_{fus}}. \quad (7)$$

During experimental studies, it was found that the values obtained at different temperatures: the

values of  $\Delta_{sol}H^{\circ}$  i  $\Delta_{sol}S^{\circ}$  were calculated in the range of temperatures listed in Table 1 and the values of  $\Delta_{fus}H^{\circ}$  were determined during the temperature melting of substances. Therefore in order to generalize the obtained results and the possibility of calculating thermodynamic parameters ( $\Delta_{mix}H^{\circ}$ ;  $\Delta_{mix}S^{\circ}$ ) at the generally accepted temperature of 298.15 K, there was a need to recalculate the values of  $\Delta_{fus}H^{\circ}$ ;  $\Delta_{fus}S^{\circ}$  up to 298.15 K. For this equations (8) and (9) were used [13]. The results of the calculation are given in the Table 3:

$$\begin{aligned} \Delta_{fus}H^{\circ}_{298.15} &= \Delta_{fus}H^{\circ}_{T_{fus}} - \\ &- \Delta_{fus}Cp^{\circ} \cdot (T_{fus} - 298.15) = \\ &= \Delta_{fus}H^{\circ}_{T_{fus}} \cdot \frac{0.35 \cdot T_{fus} + 298.15}{1.35 \cdot T_{fus}}, \end{aligned} \quad (8)$$

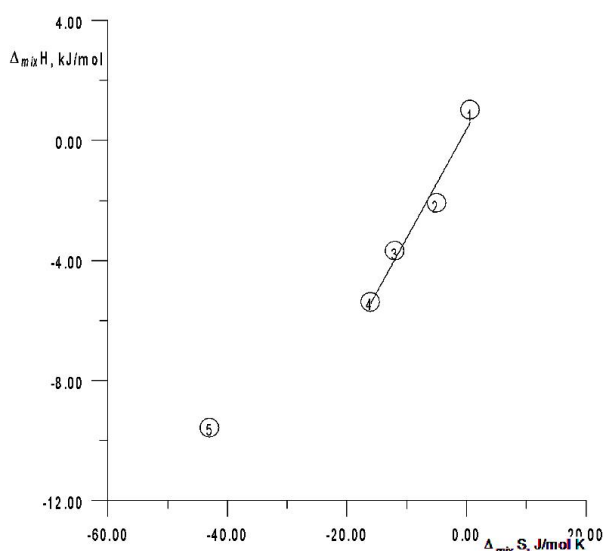
$$\begin{aligned} \Delta_{fus}S^{\circ}_{298.15} &= \Delta_{fus}S^{\circ}_{T_{fus}} - \Delta_{fus}Cp^{\circ} \cdot \ln \frac{T_{fus}}{298.15} = \\ &= \Delta_{fus}S^{\circ}_{T_{fus}} \cdot \frac{1.35 - \ln \frac{T_{fus}}{298.15}}{1.35}. \end{aligned} \quad (9)$$

The value of the change in the Gibbs energy during the mixing of components ( $\Delta_{mix}G^{\circ}$ ) at 298.15 K was calculated by equation:  $\Delta_{mix}G^{\circ} = \Delta_{mix}H^{\circ} - 298.15 \cdot \Delta_{mix}S^{\circ}$  (Table 2).

The sign and value of  $\Delta_{mix}H^p$  is determined by the change in the energy of intermolecular bonds (dispersion, orientation and hydrogen bonds) that are broken in the initial components and formed during the formation of the solution. The investigated acid has a fairly strong ( $29.0 \pm 2.5$  kJ/mol) [14] intermolecular hydrogen bonding. Therefore 5-(4-methylphenyl)-2-furanpropanoic acid in methyl and ethyl acetate, propan-1-ol and propan-2-ol, whose molecules are prone to the formation of sufficiently strong hydrogen bonds involving the carboxyl group of the acid due to the carbonyl and hydroxyl groups, does not cause a significant change in internal energy when solutions are formed. In the case of acetonitrile a significant (about 17 kJ/mol) dipole-dipole interaction between its molecules is destroyed, which is fully compensated by the formation of a hydrogen bond between the hydrogen atom of the hydroxyl group of the acid and the free electron pair on the nitrogen atom of the nitrile group in acetonitrile.

The presence of a compensatory effect of the process of mixing the acid with alcohols and acetates of equation (10) (correlation coefficient of 0.969) confirms the different types of interactions between solvents and 5-(4-methylphenyl)-2-furylpropanoic acid (Figure).

$$\Delta_{mix}H_{298} = 0.362 \cdot \Delta_{mix}S_{298} + 0.356. \quad (10)$$



Relationship between enthalpy and entropy of mixing of 5-(4-methylphenyl)-2-furanpropanoic acid in organic solvents. Points: 1 – acid solution in propan-1-ol; 2 – acid solution in propan-2-ol; 3 – acid solution in ethyl acetate; 4 – acid solution in methyl acetate; 5 – acid solution in acetonitrile

## Conclusion

The obtained thermodynamic parameters are an important source of information on the dissolution of 5-(4-methylphenyl)-2-furanpropanoic acid in organic solvents which can be used to improve production processes such as purification extraction and to increase the quality and efficiency of the substance for the synthesis of other organic compounds including pharmaceuticals.

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### **РОЗЧИННІСТЬ 5-(4-МЕТИЛФЕНІЛ)-2-ФУРАНПРОПАНОВОЇ КИСЛОТИ В ДЕЯКИХ ОРГАНІЧНИХ РОЗЧИННИКАХ**

Під час дослідження оцінено температурні залежності розчинності 5-(4-метилфеніл)-2-фуранпропанової кислоти у різних розчинниках: метил- та етилацетаті, ацетонітрилі, пропан-1-олі та пропан-2-олі. Результати аналізу подано у вигляді лінійних рівнянь за моделлю Шредера, що дало змогу визначити ентальпії, ентропії та енергії Гіббса розчинності за температури 298 К. Теплоти плавлення кислоти визначено за допомогою методу диференційно-термічного аналізу, що дало можливість розрахувати ентальпії, ентропії та енергії Гіббса змішування.

**Ключові слова:** розчинність; ентальпія розчинення; ентальпія змішування; ентальпія плавлення; 5-(4-метилфеніл)-2-фуранпропанова кислота.