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EXPERIMENTAL STUDIES OF THERMODYNAMIC PROPERTIES OF 3-(5-PHENYLPYRROL-2-YL)-PROPANOIC ACID

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For the first time, an experimental determination of the main (basic) thermodynamic properties of 3-(5-phenylpyrrol-2-yl)-propanoic acid was carried out using differential thermal and thermogravimetric methods of analysis and combustion bomb calorimetry. The values of the enthalpy of sublimation at 298 K and the enthalpy of formation in the gaseous state were calculated using the values of the enthalpies of vaporization and fusion, which were recalculated to 298 K, and the enthalpy of formation in the condensed state. The applicability of the Domalsky additive method for calculating the enthalpies of formation in the condensed and gaseous states is shown.
Thermodynamic parameters will be crucial in the development of technological processes for the synthesis, purification, use, storage and transportation of 3-(5-phenylpyrrol-2-yl)-propanoic acid, as this compound exhibit biological activity, evidenced by the preliminary assessment of the molecule structure using the web-based program SuperPred, and will have potential use in the production of medicines.

Keywords: enthalpy of formation; enthalpy of combustion; enthalpy of vaporization; enthalpy of fusion; enthalpy of sublimation.

Introduction

Various groups of organic compounds are of interest to industry and the scientific community, as they are the main or intermediate components of substances production with predetermined properties. One of such groups is polysubstituted pyrrole derivatives. The properties of pyrrole derivatives make it possible to use them in the production of dyes, catalysts, corrosion inhibitors, conductive materials for batteries, coatings for semiconductors and solar cells [1, 2]. Substances that contain a polysubstituted pyrrole fragment are quite common in nature and are usually found in the structures of

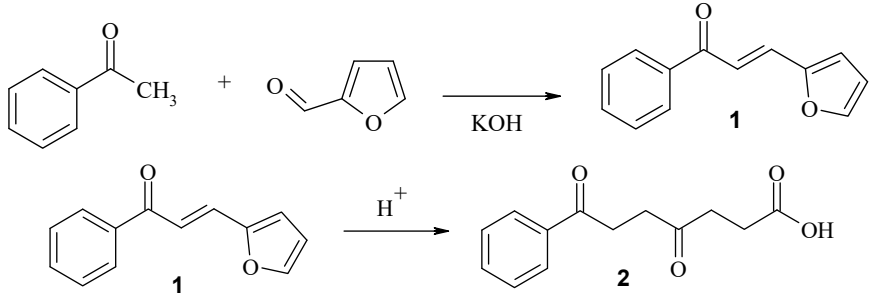
chlorophyll, hemoglobin, cytochrome [3]. Because of their biological activity, they are also used in the pharmaceutical industry. For instance, a study on a new class of 1,5-diphenyl-pyrrole derivatives indicates that these compounds can serve as excellent scaffolds for new antibacterial agents. These agents could be used on their own or as part of innovative combination therapies with existing antibiotics [4]. The presence of aromatic structure in the pyrrole molecule allows it to react with various electrophiles [5] to obtain the corresponding derivatives, which, in turn, makes it possible to use them as components in the production of medicines with antioxidant, antibacterial and anti-inflammatory effects [6]. A number of medicines contain at least one heterocycle with a nitrogen atom [7], which explains the relevance of research on new ways of synthesis and thermodynamic properties of compounds of this class.

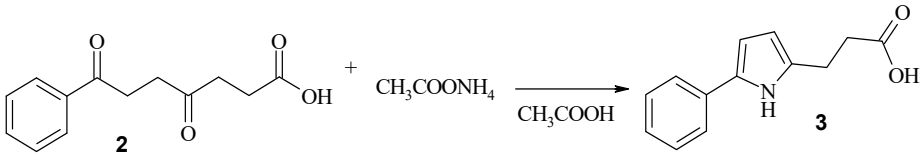
Nowadays, the development of computer technologies provides sufficient computing power to conduct a preliminary assessment of the biological activity of organic compounds, which is formed by comparing the structural formula of a substance with databases using mathematical models and machine analysis [8]. However, the lack of reliable thermodynamic data of newly synthesized compounds leads to unoptimized technological production with their application, since the important values in technological calculations of new production or optimization of existing production with the participation of individual substances are the enthalpies of phase transitions, the enthalpy of combustion of a substance $\Delta_c H^0_{298}$, the enthalpy of formation $\Delta_f H^0_{298}$ in condensed and gaseous states.

This study aims to determine the thermodynamic parameters of 3-(5-phenylpyrrole-2-yl)-propanoic acid, namely by bomb calorimetry to experimentally determine the combustion energy and calculate the enthalpy of combustion and formation in the condensed state; by differential thermal and thermogravimetric methods of analysis to determine the enthalpies of fusion ($\Delta_{fus}H_{Tfus}$) at the melting point and vaporization ($\Delta_{vap}H_{Tm}$) at the average temperature of the experimental interval and to recalculate the value of the energies of phase transitions to a temperature of 298 K and calculate the enthalpy of formation in the gaseous state at 298 K. To perform a theoretical calculation of the enthalpies of formation of 3-(5-phenylpyrrole-2-yl)-propanoic acid in the condensed and gaseous states and to compare them.

Synthesis of the compound under study

The three-step synthesis of 3-(5-phenylpyrrol-2-yl)-propanoic acid was carried out according to the following reaction scheme (Scheme 1):





Scheme 1. Reactions scheme of three-step synthesis of the 3-(5-phenylpyrrol-2-yl)-propanoic acid.

Furfurylideneacetophenone (1). To the mixture containing 80 g of furfural (0.83 mol), 100 g of acetophenone (0.83 mol), 200 mL of methanol with intense stirring was added 0.05 mol of 15 % alcohol solution of KOH. The reaction was carried out for 3 hours, maintaining the temperature from 293 to 298 K with constant stirring. Then the reaction mixture was neutralized with acetic acid, diluted in 400 mL of water, extracted with dichloromethane, the extract was washed with water on a separating funnel, the organic layer was separated and dried over sodium sulfate. The solvent was removed using a rotary evaporator and the residue was distilled under vacuum at 423.15 K / 2 mmHg.

4,7-dioxo-7-phenylheptanoic acid (2). A mixture of 0.2 mol of furfurylideneacetophenone (**1**), 300 mL of ethyl alcohol, 90 mL of concentrated HCl and 15 mL of water was refluxed for 24 hours, and then the alcohol was distilled off. To the obtained black viscous mass was added 200 mL of concentrated HCl, 200 mL of glacial acetic acid, 400 mL of water and heated with reflux condenser for another 3 hours. After cooling, the obtained light yellow crystalline precipitate of 4,7-dioxo-7-phenylheptanoic acid (**2**) was separated from the residual resin, filtered, washed three times with water and recrystallized from ethanol.

3-(5-phenylpyrrole-2-yl)-propanoic acid (3). A mixture of 0.025 mol (5.85 g) of 4,7-dioxo-7-phenylheptanoic acid (**2**), 5 g of ammonium acetate and 50 mL of glacial acetic acid was refluxed for 6 hours. After cooling, the reaction mixture was transferred under stirring to a glass with 100 mL of cold water, after 20 min the precipitate was filtered off, washed with water and recrystallized from ethanol/water mixture.

Research methods

The NMR spectroscopy method in this work was used to identify 3-(5-phenylpyrrole-2-yl)-propanoic acid. The ^{1}H NMR spectra were recorded on Varian 500 (500 MHz) using DMSO-d6 solvent. Chemical shifts (δ, ppm) are given relative to the DMSO signal (2.50 ppm): ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.15 (br.s, 1H), 10.95 (s, 1H), 7.56 (d, J = 7.5 Hz, 2H), 7.31 (t, J = 7.8 Hz, 2H), 7.09 (t, J = 7.3 Hz, 1H), 6.29 (t, J = 3.0 Hz, 1H), 5.83 (t, J = 3.0 Hz, 1H), 2.82 (t, J = 7.7 Hz, 2H), 2.57 (t, J = 7.7 Hz, 2H).

Based on the results of experimental studies carried out on the Paulik-Paulik-Erdey derivatograph Q-1500 D, the enthalpies of phase transitions were calculated. The sample of the acid under study was analysed in a platinum crucible in a dynamic mode with a heating rate of 5 K/min [9]. The value of the enthalpy of vaporization ($\Delta_{vap}H_{Tm}$) was determined from the temperature dependence of the sample vaporization rate ($v = \Delta m/\Delta\tau$) in the temperature range at which the compound was in a liquid aggregate state before the degradation process began. The integral mass loss curve was differentiated every 30 seconds, and the obtained values of the temperature dependence of the vaporization rate were analysed in the coordinates of the Arrhenius equation ($lnv =$

$A - \frac{B}{T}$, where $B = \frac{E_{act}}{R}$). To perform calculations (Eq. 1), it was assumed that the enthalpy of vaporization and the activation energy (E_{act}) of this process are equal, since in the presence of the liquid phase the process of vapor condensation is practically non-activated:

$$\Delta_{vap}H = E_{act} + RT_{fus} \quad (1)$$

As the sample loses mass, the vaporization process occurs, resulting in heat absorption. Therefore, this factor was taken into account when calculating the enthalpy of fusion (Eq. 2).

$$K \cdot S = Q_{fus} + Q_{vap} = m_0 \cdot \Delta_{fus}H + \Delta m_{vap} \cdot \Delta_{vap}H \quad (2)$$

where K is the heat transfer coefficient of the derivatograph was determined using biphenyl, silver nitrate, adipic acid, benzoic acid K-1, J/(K·s); Q_{fus} and Q_{vap} are the amount of heat absorbed during the fusion or vaporization of the sample, respectively, J; $\Delta_{fus}H$ and $\Delta_{vap}H$ are specific enthalpies of fusion and vapourisation of the acid, respectively, J/g; m_0 is the mass of the sample corresponding to the temperature of its fusion beginning T_{fus}, g; Δm_{vap} is a loss of sample mass (vapour mass) over the period taken into account when determining the peak area S (K·s) on the differential thermal analysis curve, g.

The combustion energy of 3-(5-phenylpyrrole-2-yl)-propanoic acid was measured using a precision combustion calorimeter B-08-MA with an isothermal shell (±0.003 K) and a static calorimetric bomb according to the procedure described in detail in [10]. According to the method described in [11], the energy equivalent of the calorimetric system (W = 10347±7 J/V) was determined with an accuracy of ± 0.07 % by burning reference benzoic acid of grade K-1 (the content of the main component was 99.995 ± 0.01 mol %).

The acid studied is in a solid aggregate state under normal conditions. Therefore, at the beginning of the experiment the acid was crushed in a chalcedony mortar, pressed into a tablet using a press form and placed in a platinum cup. This platinum cup was then placed in a calorimetric bomb, which was filled with oxygen. The initial pressure of oxygen, previously purified from carbon dioxide, combustible impurities and water was 30 atmospheres. At each experiment, the samples were ignited by discharging capacitors through a nichrome wire, which set the cotton thread on fire. The temperature at the beginning of the first phase in all experiments was 298.15 K. After each experiment, a by-products quantitative gas analysis of combustion was performed to detect the presence of carbon mono- and dioxide, soot, and nitric acid. The amount of carbon dioxide formed during combustion was determined by the standard Rossini method [12] with an accuracy of $\pm 2 \cdot 10^{-4}$ g.

In separate experiments, the amount of carbon monoxide was measured using indicator tubes with an accuracy of $\pm 5 \cdot 10^{-6}$ g. The reliability of gas analysis is confirmed by numerous experiments on the combustion of reference benzoic acid. The presence of HNO_3 was determined by titration with 0.1N KOH. The amount of soot formed on the walls of the platinum cup after the acid combustion experiment was determined by weighing with an accuracy of $\pm 5 \cdot 10^{-6}$ g.

Results and discussion

The synthesized acid belongs to pyrrole derivatives, compounds of which are capable of exhibiting biological activity. For this reason, an additional preliminary assessment of

the potential biological activity was performed using the web-based program SuperPred [13]. The assessment is based on the comparing the structural similarity between the substance under study (in this case, an acid) and biotarget ligands, as well as the probability of ligand-receptor interaction (the evaluation database contains about 1800 proteins, 340 thousand ligand compounds and information on 660 thousand interactions between compounds and targets). According to the results of preliminary evaluation, 3-(5-phenylpyrrole-2-yl)-propanoic acid is capable of exhibiting biological activity. When targeting cathepsin D protein, the probability of the drug's effect on arterial hypertension [ICD-11: BA00-BA04] and multiple sclerosis [ICD-11: 8A40] is 96.0%, the same as for most drugs with a pyrrole fragment [14]. Targeting a membrane protein (toll-like receptor 8) has a 64.7% probability of producing a therapeutic effect in allergic rhinitis [ICD-11: CA08.0] and systemic lupus erythematosus [ICD-11: 4A40.0]. The effect on the enzyme DNA topoisomerase I will be observed in 82.3% of cases of chemotherapeutic effect in such cancers as acute lymphoblastic leukemia [ICD-11: 2A85], lung cancer [ICD-11: 2C25. 0] and esophageal cancer [ICD-11: 2B70], as well as in acquired immunodeficiency syndrome [ICD-11: 1C62.3] and bacterial infection [ICD-11: 1A00-1C4Z]. When acting on M5 muscarinic acetylcholine receptors, there is an 88.0% probability that the drug will have a therapeutic effect in the treatment of allergic rhinitis [ICD-11: CA08.0]; Alzheimer's disease [ICD-11: 8A20]; asthma [ICD-11: CA23]; colitis [ICD-11: 1A40.Z]; gastritis [ICD-11: DA42]. The accuracy of the SuperPred forecasting method is 99.0-95.0 %. According to these results of preliminary assessment, 3-(5-phenylpyrrole-2-yl)-propanoic acid is a potential component of medicines with a wide range of biological activity.

The values of the enthalpies of vaporization calculated by Eq. 1 are given in Table 1.

Table 1

Vapourisation enthalpies of 3-(5-phenylpyrrol-2-yl)-propanoic acid

Sample number	T_1-T_2, K	$\sum\Delta m \cdot 10^3$, g	A	-B, K	$\Delta_{vap}H$, kJ/mol
1	451.6-470.1	0.154	13.99	11553	99.5
2	485.4-540.1	3.430	13.30	11447	98.6
3	440.4-540.8	7.130	14.37	11605	99.9
Mean value:					99.3±1.0

T_1-T_2 – the temperature interval at which the enthalpy of vapourisation is calculated;
$\Sigma\Delta m$ – total mass loss of the sample at the specified temperature interval, g.

The values of the enthalpies of fusion calculated using Eq. 2 are shown in Table 2.

Table 2

Fusion enthalpies of 3-(5-phenylpyrrol-2-yl)-propanoic acid

Sample number	m_0, g	Δm_{vap}, g	S, K·s	q_{vap}, J	$K \cdot 10^3$, J/K·s	$\Delta_{fus}H$, kJ/mol
T_{fus}= 416.45±1.50 K;						
1	0.0746	0.0003	306.9	0,1428	3.574	29.28
2	0.0740	0.0003	306.7	0.1406	3.804	28.25
3	0.1012	0.0004	399.1	0.1818	3.104	28.60
Mean value:						28.71±0.78

The experimental determination of the combustion energy of the studied acid was carried out according to the method [11]. Under the experimental conditions, the combustion energy ($Q_{V(298)}$) was calculated by Eq. 3:

$$-Q_{V(298)} = \frac{W \cdot \Delta T - Q_{fuser} - Q_{HNO_3} + Q_{carb}}{m_{comp}} \quad (3)$$

where W is an energy equivalent of the calorimetric system, J/V; m_{comp} – is a mass of the substance that was burned during the experiment, g; Q_{fuser}, Q_{HNO3}, Q_{carb} are the amount of heat released during the combustion of cotton thread (16704.2 J/g), in the formation of nitric acid solution (59 J/g) and soot formation (32800 J/g), respectively [11]; ΔT is a true temperature rise in a calorimetric experiment.

The completeness of combustion after burning the acid sample was calculated as the ratio of the mass of carbon dioxide determined by gas analysis ($m_{CO_2}^{exp}$) to the mass of carbon dioxide calculated from the sample taken for the study ($m_{CO_2}^{calc}$). The experimental determination of the combustion energy and completeness of acid combustion results are shown in Table 3.

Table 3

Results of experimental determination of 3-(5-phenylpyrrol-2-yl)-propanoic acid combustion energies

m_{comp}, g	ΔT, V	Q_{fuser}, J	Q_{HNO_3}, J	Q_{carb}, J	$-Q_{V(298)}$, J/g	$m_{CO_2}^{exp} / m_{CO_2}^{calc}$
0.23751	0.70868	79.1	4.1	22.1	30619	0.9954
0.23877	0.71561	97.6	8.9	11.8	30618	0.9982
0.21210	0.63366	88.5	1.8	21.6	30591	0.9912
0.29435	0.87748	87.7	3.0	19.5	30606	0.9946
0.27742	0.82594	79.8	4.1	23.0	30589	0.9989
0.30872	0.91955	87.9	4.4	22.6	30597	0.9975
0.12968	0.38956	87.1	2.4	25.9	30596	0.9937
$\Delta Q_{V(298)}$ = –30602±11 J/g						

The mean value of the combustion energy was used to further calculate the standard enthalpy of combustion of 3-(5-phenylpyrrol-2-yl)-propanoic acid. The value of the standard enthalpy of combustion was calculated taking into account the Washburn correction π [11] and the correction for the expansion work ΔnRT. The following values of formation energies (kJ/mol) were used to calculate the standard enthalpy of formation $\Delta_f H_{298}^0$ in the condensed state by the combustion reaction (Eq. 4): CO_2(g) = 393.51±0.13; H_2O(l) = 285.830±0.040; O_2(g) = 0; N_2(g) = 0 [15].

$$C_{13}H_{13}O_2N\ (cr) + 15.25O_2\ (g) \rightarrow 13CO_2\ (g) + 6.5H_2O\ (l) + 0.5N_2\ (g) \quad (4)$$

The energy of combustion, the Washburn correction, the correction for the expansion work and the enthalpy properties of the acid are given in Table 4.

Table 4

Energy characteristics of combustion and formation (kJ/mol)
3-(5-phenylpyrrol-2-yl)-propanoic acid in condensed and gaseous states

$Q_{V(298)}$	π	ΔnRT	$\Delta_c H^0_{298}$	$\Delta_f H^0_{298}$,(cr)	$\Delta_f H^0_{298}$, (g)
–6587.2±2.3	–4.1	–4.3	–6595.6±2.3	–377.9±2.6	–243.3±3.3

To calculate the enthalpies of formation in the gaseous state, the value of the enthalpy of sublimation at 298 K is required. The value of the enthalpy of sublimation can be calculated from the values of the enthalpies of fusion and vaporization, with its subsequent reduction to 298 K. For the purpose of reducing the error of recalculation of the enthalpy of sublimation to 298 K, we decided to recalculate the value of the enthalpy of sublimation from the melting point to 298 K according to Eq. 5, in which the value of the change in the specific heat capacity during the melting process is presented as a constant value (0.259 ± 0.041) [16].

$$\Delta_{sub}H_{298} = \Delta_{sub}H_{T_{fus}} + (0.259 \pm 0.041) \cdot M \cdot \left(T_{fus} - 298\right) \quad (5)$$

Assuming that the value of the enthalpy of fusion is determined at the melting point and the enthalpy of vaporization is determined at the temperature range close to the melting point. The enthalpy of sublimation was determined at the melting point ($\Delta_{sub}H_{T_{fus}}$).

The value of the enthalpy of sublimation at 298 K is 134.6±2.1 kJ/mol, respectively, the value of the enthalpy of formation of 3-(5-phenylpyrrole-2-yl)-propanoic acid in the gaseous state is $\Delta_f H^0_{298}$, (g) = –243.3 ± 3.3 kJ/mol.

The presented algorithm for determining the thermodynamic parameters of individual substances experimentally is a complex process that requires particularly pure substances, expensive precision equipment, and highly qualified scientists. An alternative to this is theoretical methods for calculating the main thermodynamic parameters. Such methods are usually able to provide sufficient reproducibility results for compounds with a simple structure. The simplest additive calculation methods are Benson [17], Cohen [18] and Domalski [19]. Benson group additivity method is the primary method that makes it possible to calculate the enthalpies of formation in the gaseous state from group contributions, but its main drawback is that the group contributions of this method are scattered in scientific publications, access to which is limited and allows calculating only the enthalpies of formation in the gaseous state. Cohen's method allows us to calculate thermodynamic parameters only for those compounds that consist of carbon, oxygen, and hydrogen. The Domalsky additive method can be used to calculate the enthalpies of formation in the condensed and gaseous states simultaneously, and group contributions are not scattered across publications but are concentrated in [19]. Table 5 shows all the necessary group contributions to calculate the enthalpies of formation of 3-(5-phenylpyrrol-2-yl)-propanoic acid.

Based on the Domalsky method, the enthalpy of formation in the condensed state is $\Delta_f H^0_{298}$ (cr) = – 377.61 kJ/mol, and in the gaseous state $\Delta_f H^0_{298}$ (g) = –240.93 kJ/mol. Theoretically calculated values by the Domalsky method are in good agreement with experimental data. Such a convergence of values may be caused by the spatial structure of the substance under study, namely, the presence of large substituents that reduce the

possibility of intra- and intermolecular interactions that cause significant differences between experimentally and analytically determined values.

Table 5

Group contributions for Domalsky method calculations of enthalpies of formation in condensed and gaseous states, kJ/mol

Group	$\Delta_f H^0_{298}$		Group	$\Delta_f H^0_{298}$	
	(cr)	(g)		(cr)	(g)
$C_b – (C_b)_2(H)$	6.53	13.81	$C_d – (C_d)(C)(N)$	–3.95	–5.74
$C_b – (C_d)(C_b)_2$	20.27	24.17	$C – (C)(C_d)(H)_2$	–21.6	–18.92
$C_d – (C_b)(C_d)(N)$	–3.95	–5.74	$C – (C)(CO)(H)_2$	–27.9	–21.84
$C_d – (C_d)_2(H)$	17.53	28.28	CO – (C)(O)	–153.6	–137.24
$N – (C_d)_2(H)$	45.40	83.55	O – (CO)(H)	–282.15	–254.30
$C_b – (C_b)_2(N)$	9.75	–1.30	Pyrrole ring	–17.84	–30.48

Conclusions

The thermodynamic properties of 3-(5-phenylpyrrole-2-yl)-propanoic acid were determined by experimental methods. The values of the enthalpy of combustion (-6595.6 ± 2.3 kJ/mol) and formation in the condensed state (–377.9 ± 2.6 kJ/mol) were determined experimentally by bomb calorimetry. The differential thermal analysis method was used to determine the enthalpy of fusion (28.71 ± 0.78 kJ/mol) at the melting point of 416.45 ± 1.50 K and to calculate the value of the enthalpy of vaporization (99.3 ± 1.0 kJ/mol). Using the experimentally determined enthalpies of phase transitions, the value of the enthalpy of sublimation was calculated and recalculated to 298 K (134.6 ± 2.1 kJ/mol). The enthalpy of formation in the gaseous state is calculated (–243.3 ± 3.3 kJ/mol). The Domalsky additive method was used as a theoretical method for calculation the main thermodynamic parameters of 3-(5-phenylpyrrole-2-yl)-propanoic acid. A theoretical values of enthalpies of formation in the condensed and gaseous states ($\Delta_f H^0_{298}$ (cr) = –377.61 kJ/mol and $\Delta_f H^0_{298}$ (g) = –240.93 kJ/mol, respectively) are in good agreement with experimental data

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РЕЗЮМЕ

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ЕКСПЕРИМЕНТАЛЬНЕ ВИЗНАЧЕННЯ ТЕРМОДИНАМІЧНИХ ВЛАСТИВОСТЕЙ 3-(5-ФЕНІЛПІРОЛ-2-ІЛ)-ПРОПАНОВОЇ КИСЛОТИ

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3-(5-фенілпірол-2-іл)-пропанова кислота є представником групи похідних полізаміщеного піролу і здатна проявляти біологічну активність, про що свідчить попередня оцінка структури молекули за допомогою веб-програми SuperPred. Подібні речовини застосовуються у фармацевтичній промисловості у якості основних або проміжних компонентів для виробництв лікарських засобів з антиоксидантною, антибактеріальною та протизапальною діями. Попри актуальність пошуку нових шляхів синтезу речовин, відсутність надійних термодинамічних даних зумовлює потребу у їх наявності, оскільки вони є одними з ключових складових під час технологічних розрахунків процесів синтезу, очищення, використання, зберігання та транспортування за участю індивідуальних речовин.

Ентальпії спалювання ($\Delta_c H^0_{298}$ =–6595,6 ± 2,3 кДж/моль) та утворення в конденсованому стані ($\Delta_f H^0_{298}$ (cr) =-377,9 ± 2,6 кДж/моль) були визначені експериментально методом бомбової калориметрії.

Ентальпія плавлення ($\Delta_{fus} H^0$ = 28,71 ± 0,78 кДж/моль) при температурі плавлення 416,45 ± 1,50 K була визначена методом диференціального термічного аналізу. Використовуючи це значення, ентальпія випаровування ($\Delta_{vap} H^0$ = 99,3 ± 1,0 кДж/моль) була розрахована. За визначеними ентальпіями фазових переходів розраховано значення ентальпії сублімації з подальшим перерахунком до 298 K ($\Delta_{sub} H^0_{298}$ = 134,6 ± 2,1 кДж/моль). На основі ентальпії сублімації було розраховано ентальпію утворення в газоподібному стані ($\Delta_f H^0_{298}$(g) = –243,3 ± 3,3 кДж/моль).

Адитивний метод Домальського використано як теоретичний метод розрахунку основних термодинамічних параметрів 3-(5-фенілпірол-2-іл)-пропанової кислоти, а саме ентальпії утворення в конденсованому ($\Delta_f H^0_{298}$ (cr) = – 377,61 кДж/моль) та газоподібному станах ($\Delta_f H^0_{298}$ (g) = –240,93 кДж/моль). Розраховані теоретичні значення добре узгоджуються з експериментальними даними.

Ключові слова: ентальпія утворення; ентальпія спалювання; ентальпія випаровування; ентальпія плавлення; ентальпія сублімації.

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