D. S. Shevchenko[1], Y. I. Horak[2], N. I. Tischenko[3], D. B. Pyshna[1], I. B. Sobechko[1]

[1] Lviv Polytechnic National University,
Department of Physical, Analytical and General Chemistry
[2] Ivan Franko National University of Lviv,
Department of Organic Chemistry
[3] Frantsevich Institute for Problems of Materials Science NASU
Department of Physics, Chemistry and Technology of Nanotextured Ceramics and Nanocomposite Materials
[1] dmytro.s.shevchenko@lpnu.ua

THERMODYNAMIC PROPERTIES OF
3-(1,5-DIPHENYLPYRROL-2-YL)-PROPANOIC ACID

Using precision equipment, the enthalpies of vaporization, fusion and formation in the condensed state of 3-(1,5-diphenylpyrrol-2-yl)-propanoic acid were experimentally determined. The enthalpy of sublimation at 298 K and the enthalpy of formation in the gaseous state were calculated. A comparative analysis of the experimentally determined values with theoretically calculated values using additive calculation methods is given.

Key words: combustion energy; enthalpy of combustion; enthalpy of formation; enthalpy of vaporization; enthalpy of fusion; 3-(1,5-diphenylpyrrol-2-yl)-propanoic acid.

Introduction

The presence in nature of organic substances containing pyrrole fragments with various substituents in the ring and the diversity of properties in such compounds is of interest to the scientific community and industry, in particular. Substances with a pyrrole fragment are usually found in the structures of hemoglobin, cytochrome, chlorophyll, etc. [1]. Pyrrole derivatives are a group of substances with a wide range of applications in industry. Compounds of this class are used in the production of dyes, catalysts, corrosion inhibitors, as conductive materials in battery production, as coatings for semiconductors and solar cells [2, 3]. The pharmaceutical industry also pays attention to such organic substances, as heterocyclic compounds with a nitrogen heteroatom have useful biological activity, which makes it possible to use them as components of medicines with antioxidant, antibacterial, and anti-inflammatory effects [4]. Such a variety of biological activity is explained by the presence of an aromatic structure in the pyrrole, which allows it to react with different electrophiles [5].

The fact that such a range of biological activity is present motivates to investigate the ways of synthesis of new poly-substituted pyrrole derivatives. One of such synthesized derivatives is 3-(1,5-diphenylpyrrole-2-yl)-propanoic acid. Although the current progress in computer technology [6] makes it possible to carry out a preliminary assessment of organic compounds for biological activity by comparing the structural formula of a substance with databases, there is a necessity to have reliable thermodynamic data of newly synthesized compounds. The values of the enthalpies of combustion of substances $\Delta_c H^0_{298}$ are an important thermochemical parameter, as theyallow to characterize the energy of internal and intermolecular interactions. The enthalpies of formation values calculated using enthalpies of combustion values $\Delta_f H^0_{298}$ in condensed and gaseous states are key parameters in thermodynamic calculations of chemical processes involving individual substances. **The purpose of this paper** is to determine the energy of combustion of 3-(1,5-diphenylpyrrol-2-yl)-propanoic acid using the bomb calorimetry method and calculate the enthalpies of combustion and formation in the condensed state. Determine phase transition energies by differential thermal and thermogravimetric analysis. Convert phase transition energy values to the standard temperature of 298 K

and calculate the enthalpy of formation in the gas phase. To perform an analytical calculation of the thermodynamic parameters of 3-(1,5-diphenylpyrrol-2-yl)-propanoic acid and compare the obtained values with the experimentally determined ones.

Materials and research methods

Reactions for the synthesis of 3-(1,5-diphenyl-pyrrole-2-yl)-propanoic acid were carried out according to the following scheme (Fig. 1) in three stages:
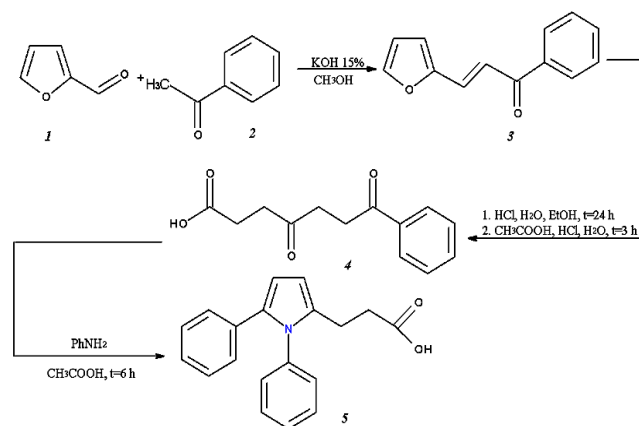

*Fig. 1. The synthesis scheme
of the 3-(1,5-diphenylpyrrol-2-yl)-propanoic acid*

At the first stage, to the reaction mixture (furfural (**1**) 80 g, acetophenone (**2**) 100 g, methanol 200 mL) under intense stirring 0.05 mol 15 % solution of KOH was added. Stirring for 3 hours, the temperature of the reaction mixture was maintained in the range of 293–298 K. After that, the reaction mixture was neutralized with acetic acid, diluted in 400 mL of water, extracted with dichloromethane, washed with water, the organic layer was separated and dried with sodium sulfate. The solvent was removed and the residue was distilled in a vacuum. Hence, furfurylideneacetophenone (**3**) was obtained. In the second stage, 0.2 mol of furfurylidenea-cetophenone (**3**), 300 mL of ethyl alcohol, 90 mL of concentrated HCl and 15 mL of water were mixed. The prepared mixture was boiled with reflux for 24 hours, after which the alcohol was distilled off. To the obtained black viscous mass 200 mL of concentrated HCl, 200 mL of ice-cold acetic acid, 400 mL of water were added and heated under reflux for another 3 hours. After cooling, the resulting light-yellow crystalline precipitate of 4,7-dioxo-7-phenylheptanoic acid (**4**) was decanted from the

residual resin, filtered, washed three times with water, and recrystallized from ethanol. In the third step, the synthesized 4,7-dioxo-7-phenylheptanoic acid (**4**) was mixed in an amount of 0.025 mol (5.85 g) with 0.025 mol of aniline and 50 mL of ice-cold acetic acid. This mixture was refluxed for 6 hours. After cooling, the reaction mixture was transferred under stirring to a flask with 100 mL of cold water. After 20 min, the resulting precipitate was filtered off, washed with water, and recrystallized from an ethanol/dimethylformamide mixture.

The identification of 3-(1,5-diphenylpyrrole-2-yl)-propanoic acid was performed using NMR spectroscopy. The ^{1}H NMR spectra were recorded on Varian 500 (500 MHz) using solvent DMSO-d6 solvent. Chemical shifts (δ, ppm) are given relative to the DMSO signal (2.50 ppm): ^{1}H NMR (500 MHz, DMSO-d6) δ 12,14 (br.s, 1H); 7.49–7.37 (*m*, 3H); 7.21 (*d*, *J* = 7.3 Hz, 2H); 7.13 (*t*, *J* = 7.5 Hz, 2H); 7.06 (*t*, *J* = 7.3 Hz 1H); 7.00 (*d*, *J* = 7.2 Hz, 2H); 6.33 (*d*, *J* = 3.6 Hz, 1H); 6.07 (*d*, *J* = 3.6 Hz, 1H); 2.60 (*t*, *J* = 7.7 Hz, 2H); 2.43 (*t*, *J* = 7.7 Hz, 2H).

The enthalpies of phase transitions were calculated based on the results of experimental studies on the Q-1500 D derivatograph of the Paulik – Paulik –Erdey system. The sample was analyzed in a platinum crucible in dynamic mode at a heating rate of 5 K/min [7]. The enthalpy of vaporization value ($\Delta_{vap}H$) was determined from the temperature dependence of the sample vapor rate $v = \Delta m/\Delta \tau$ in the temperature range where the compound was in the 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 vapourization rate were analyzed in the coordinates of the Arrhenius equation ($lnv = A - B/T$, where $B = E_{act}/R$). Since vapor condensation in the presence of a liquid phase is practically an activation-free process, it was assumed that the enthalpy of vaporization and the activation energy (E_{act}) of this process were equal (Eq. (1)):

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

The calculation of the enthalpy of fusion ($\Delta_{fus}H_{T_{fus}}$) was performed taking into account the heat absorbed during the vaporization of the loss of sample mass, Eq. (2):

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

where K is the heat transfer coefficient of the derivatograph was determined using biphenyl, silver nitrate, adipic acid, and benzoic acid K-1 and was $8.2023 \cdot 10^{-5} \cdot T_{fus}$, 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 vapourization 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 (vapor 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-(1,5-diphenyl-pyrrole-2-yl)-propanoic acid was measured using a precision combustion calorimeter B-08-MA with a shell (±0.003 K) and a static calorimetric bomb according to the procedure described in detail in [8].The energy equivalent of the calorimetric system ($W = 10347 \pm 7$ J/V) was determined according to the procedures given in [9] with an accuracy of ±0.06 %, burning the reference benzoic acid of the K-1 brand, the content of the main component of which reached 99.995 ± 0.01 mol. %.

Under normal conditions, acid being investigated existed in a solid aggregate form. At the beginning of the experiment, it was powdered in a chalcedony mortar, formed into tablets using a press mold, and placed in a platinum cup. During the experiment, the samples were ignited by discharging capacitors through a nichrome wire, which set fire to a cotton thread. The initial pressure of oxygen, pre-purified from combustible impurities, carbon dioxide, and water, was 30 atmospheres. The temperature at the beginning of the primary phase in all experiments was 298.15 K.

Following each combustion, the combustion by products underwent a quantitative analysis to detect the presence of mono- and dioxide, soot, and nitric acid. To determine the amount of carbon dioxide formed during combustion Rossini method [10] was used with an accuracy of $\pm 2 \cdot 10^{-4}$ g. The carbon monoxide content was measured in separate experiments using indicator tubes with an accuracy of $\pm 5 \cdot 10^{-6}$ g. The reliability of the gas analysis has been confirmed by numerous combustion experiments of reference benzoic acid. The amount of soot formed on the walls of the platinum cup after burning the acid was determined by weighing with an accuracy of $\pm 5 \cdot 10^{-6}$ g. The HNO_3 presence was analyzed by titration with 0.1 N KOH.

Results and discussion

Since the synthesized acid belongs to the pyrrole derivatives which are capable of exhibiting biological activity, a preliminary assessment of the potential biological activity was carried out using the web-based software Super Pred [11]. The assessment is based on a comparison of the structural similarity between the substance under investigation (in this case, an acid) and biotarget ligands, as well as the probability of ligand-receptor interaction (the database for the assessment includes 1800 proteins, 340 thousand ligand compounds, and information on 660 thousand interactions between compounds and targets).

In the case of 3-(1,5-diphenylpyrrole-2-yl)-propanoic acid effect on cathepsin D protein, the drug effect on hypertension [ICD-11: BA00-BA04] and multiple sclerosis [ICD-11: 8A40] is 96.7 % likely to occur, as in most drugs with a pyrrole fragment [12]. When acting on the muscarinic acetylcholine receptor M5, there is a 71.4 % probability of a medicinal effect in 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]. When targeting a membrane protein (toll-like receptor 8), 81.3 % of patients will have a therapeutic effect on allergic rhinitis [ICD-11: CA08.0] and systemic lupus erythematosus [ICD-11: 4A40.0]. The effect on the DNA topoisomerase I enzyme will be shown in 78.1 % of cases of chemotherapeutic effect in such cancers as acute lymphoblastic leukemia [ICD-11: 2A85], lung cancer [ICD-11: 2C25.0] and oesopha-geal cancer [ICD-11: 2B70], as well as acquired immunodeficiency syndrome [ICD-11: 1C62.3] and bacterial infection [ICD-11: 1A00-1C4Z]. The accuracy of the forecasting method is 99.0–94.6 %.

According to the results of analytical studies, 3-(1,5-diphenylpyrrole-2-yl)-propanoic acid is a potential component of medicines with a wide range of biological activity.

The values of the vapourization and melting enthalpies calculated from Eq. (1) and (2) are given in Table 1.

The experimental determination of the combustion energy of the investigated acid was carried out according to the previously described procedure. The combustion energy ($Q_{V(298)}$) under the experimental conditions was calculated according to 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 [9]; ΔT is a true temperature rise in a calorimetric experiment.

The results of determining the combustion energy of the acid and the completeness of its combustion are shown in Table 2. The completeness of combustion was calculated as the ratio of the mass of carbon dioxide determined by the results of gas analysis ($m_{CO_2}^{exp}$), to the mass of carbon dioxide calculated from the initial sample taken for the study ($m_{CO_2}^{calc}$).

Table 1

Fusion and vapourization enthalpies of 3-(1,5-diphenylpyrrol-2-yl)-propanoic acid

Sample number	m_0, g	Δm_{vap}, g	S, K·s	q_{vap}, J	$\Delta_{fus}H$, kJ/mol	$\delta(\Delta_{fus}H)$, %	T_1-T_2, K	$\sum \Delta m \cdot 10^3$ g	A	$-B$, K	$\Delta_{vap}H$, kJ/mol	$\delta(\Delta_{vap}H)$, %
T_{fus}= 442.4±1.5 K; K = 0.03628 J/K·s											
1	0.1009	0.0013	436.9	0.4813	44.4	1.83	522.6–600.8	35.7	24.08	12445	107.10	0.09
2	0.1096	0.0013	456.9	0.4621	42.8	1.83	511.2–593.8	11.2	23.10	12414	106.90	0.09
	Mean value:				43.6±1.2				Mean value:		107.00±0.14	

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

Table 2

Results of experimental determination of the combustion energies of 3-(1,5-diphenylpyrrol-2-yl)-propanoic acid

m_{comp}, g	ΔT, V	Q_{fuser}, J	Q_{HNO_3}, J	Q_{carb}, J	$-Q_{V(298)}$, J/g	$\delta(Q_{V(298)})$, %	$m_{CO_2}^{exp}/m_{CO_2}^{calc}$
0.29835	0.95757	92.7	8.6	20.5	32942	0.04	0.9998
0.29265	0.93708	71.3	3.2	31.0	32986	0.08	0.9958
0.29763	0.95427	91.3	5.0	31.0	32959	0.00	0.9975
0.28733	0.92117	89.3	6.8	40.0	32981	0.07	0.9966
0.21690	0.69961	95.2	1.2	8.2	32971	0.04	0.9969
0.29885	0.95591	72.7	4.1	21.6	32915	0.13	0.9996
0.22445	0.72207	81.0	1.5	6.6	32952	0.01	0.9986
$\otimes Q_{V(298)}$= –32958±16 J/g							

Based on the experiments, the mean value of the combustion energy was used to calculate the value of the standard enthalpy of combustion $\Delta_c H_{298}^0$ of the acid under investigation. The value of the standard enthalpy of combustion of the acid under

study was calculated taking into account the Washburn correction π [9] 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 $\Delta_f H^0_{298}$ in the condensed state by the combustion reaction: CO_2 (g) = 393.51±0.13; H_2O (l) = 285.830±0.040; O_2 (g) = 0 [13]. The energy

of combustion, the Washburn correction, the correction for the expansion work, and the enthalpy properties of the acid under study are given in Table 3.

Energy characteristics of combustion and formation
3-(1,5-diphenylpyrrol-2-yl)-propanoic acid in condensed and gaseous states, kJ/mol

$Q_{V(298)}$	π	ΔnRT	$\Delta_c H^0_{298}$	$\Delta_f H^0_{298, \text{ cr}}$	$\Delta_f H^0_{298, \text{ g}}$
−9602.3 ± 4.7	−6.1	−6.8	−9615.2 ± 4.7	−291.1 ± 4.7	−129.5 ± 5.5

In order to summarize the results and calculate the enthalpies of sublimation to determine the enthalpies of formation in the gaseous state, it is necessary to recalculate the enthalpies of phase transitions to 298 K. For this recalculation, the values of the change in heat capacity (ΔC_p) at the corresponding phase transition are required. Since experimental methods require expensive and specialized equipment to determine the heat capacity, analytical calculation methods are often used. The method of additive group contributions by Chickos and Acree [14] is most commonly used, but the results of the recalculation using a much simpler method developed by scientists at Lviv Polytechnic are the same within the calculation errors of both methods [8]. Therefore, the enthalpy of sublimation was recalculated using equation (4), assuming that the enthalpy of sublimation value ($\Delta_{sub} H_{T_{fus}}$) is calculated as the sum of the enthalpy of vapourization ($\Delta_{vap} H_{T_{fus}}$) and enthalpy of fusion ($\Delta_{fus} H_{T_{fus}}$).

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

(4)

Hence, the enthalpy of sublimation value at 298 K is equal to 161.5±2.9 kJ/mol, and taking into account this value, the enthalpy of formation of 3-(1,5-diphenylpyrrol-2-yl)-propanoic acid in the gaseous state in $\Delta_f H^0_{298}$ (g) = –129.5±5.5 kJ/mol.

The experimental procedures described above for determining thermodynamic parameters are complex and expensive, requiring precision equipment and highly skilled researchers. For this reason, special attention should be paid to alternative approaches to calculating these parameters. Among the simplest are the group contribution methods, which include the methods of Benson [15], Domalski [16], Cohen [17], Salmon [18]. These methods generally provide a good reproducibility of results for compounds with simple structures. Since the acid under study is a complex compound with a heteroatom nitrogen, it is impossible to calculate its thermodynamic parameters using the Benson and Cohen methods. The Benson method has a limited number of nitrogen-containing group contributions that describe the compound under study, while the Cohen method allows calculating the thermodynamic parameters of compounds containing only carbon, oxygen, and hydrogen.

Group contributions for calculation of enthalpies of formation in solid and gaseous state, kJ/mol

Group	$\Delta_f H^0_{298}$			Group	$\Delta_f H^0_{298}$		
	Salmon [18]	Domalski [16]			Salmon [18]	Domalski [16]	
	(cr)	(cr)	(g)		(cr)	(cr)	(g)
$C_b – (C_b)_2(H)$	3.1	6.53	13.81	$C_d – (C_d)(C)(N)$	−74.3	−3.95	−5.74
$C_b – (C_d)(C_b)_2$	60.2	20.27	24.17	$C – (C)(C_d)(H)_2$	10.6	−21.6	−18.92
$C_d – (C_b)(C_d)(N)$	1.9	−3.95	−5.74	$C – (C)(CO)(H)_2$	−70.9	−27.9	−21.84
$C_d – (C_d)_2(H)$	18.3	17.53	28.28	$CO – (C)(O)$	−183.1	−153.6	−137.24
$N – (C_d)_2(C_b)$	−18.1	88.92	120.64	$O – (CO)(H)$	−212.4	−282.15	−254.3
$C_b – (C_b)_2(N)$	62.0	9.75	−1.3	Pyrrole ring	−21.0	−17.84	−30.48

We have therefore used the Domalski method to calculate the enthalpies of formation of the acid in the condensed (solid) and gaseous states, and the Salmon method to calculate the enthalpy of formation in the condensed state. All required group contributions are presented in Table 4.

According to the Salmon method, the enthalpy of formation in the condensed state is –377.5 kJ/mol. The difference between the experimentally determined value and the calculated one is 86.4 kJ/mol. Regarding the values calculated by the Domalski method $\Delta_f H^0_{298}$,(cr) = –291.7 kJ/mol and $\Delta_f H^0_{298}$, (g) = –136.1 kJ/mol, these values are in full agreement with the experimental ones. Such agreement between the results of the analytical calculation method and the experimentally determined may be due to the spatial structure of the acid. For instance, the presence of two phenyl rings in the fifth and first positions of the pyrrole ring hinders the formation of intra- and intermolecular interactions in the molecule, which have a significant impact on the thermodynamic properties of individual substances.

Conclusions

As a result of the studies, the enthalpies of combustion ((–9615.2 ± 4.7) kJ/mol) and formation in the condensed state ((–291.1 ± 4.7) kJ/mol) of 3-(1,5-diphenylpyrrol-2-yl)-propanoic acid were determined experimentally. By the differential thermal method of analysis, the enthalpy of fusion at a melting point of 442.4 K ((43.6 ± 1.2) kJ/mol) was calculated. The value of the enthalpy of vapourisation ((107.00 ± 0.14) kJ/mol) was calculated by the thermogravimetric method of analysis. Based on the experimentally determined enthalpies of phase transitions, the value of the enthalpy of sublimation was calculated and recalculated to 298 K. Enthalpy of formation in the gaseous state was calculated ((–129.5 ± 5.5) kJ/mol). The possibility of applying the additive Domalski method to calculate the enthalpies of formation in the condensed and gaseous states is shown.

References

1. Ribeiro da Silva, M. A., & Santos, A. F. (2010). Calorimetric and computational study of 2- and 3-acetyl-1-methylpyrrole isomers. *The Journal of Physical Chemistry B*, 114(8), 2846–2851. https://doi.org/10.1021/jp911323c

2. Santos, A. F., & Ribeiro da Silva, M. A. (2013). Molecular energetics of alkyl pyrrolecarboxylates: Calorimetric and computational study. The Journal of Physical Chemistry A, 117(24), 5195–5204. https://doi.org/10.1021/jp4032628

3. Santos, A. F., & Ribeiro da Silva, M. A. V. (2014). Experimental and high level ab initio enthalpies of formation of di- tri- tetra- and pentamethyl- substituted pyrroles. *The Journal of Chemical Thermodynamics*, 75, 1–7. https://doi.org/10.1016/j.jct.2014.04.003

4. Santos, A. F., & Ribeiro da Silva, M. A. V. (2010). A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives. *The Journal of Chemical Thermodynamics*, 42(12), 1441–1450. https://doi.org/10.1016/j.jct.2010.06.012

5. Ivan, B.-C., Barbuceanu, S.-F., Hotnog, C. M., Anghel, A. I., Ancuceanu, R. V., Mihaila, M. A., Brasoveanu, L. I., Shova, S., Draghici, C., Olaru, O. T., Nitulescu, G. M., Dinu, M., & Dumitrascu, F. (2022). New pyrrole derivatives as promising biological agents: Design, synthesis, characterization, in silico, and cytotoxicity evaluation. *International Journal of Molecular Sciences*, 23(16), 8854. https://doi.org/10.3390/ijms23168854

6. Forouzesh, A., Samadi Foroushani, S., Forouzesh, F., & Zand, E. (2019). Reliable target prediction of bioactive molecules based on chemical similarity without employing statistical methods. *Frontiers in Pharmacology*, 10. https://doi.org/10.3389/fphar.2019.00835

7. Klachko, O., Matiychuk, V., Sobechko, I., Serheyev, V., & Tishchenko, N. (2020). Thermodynamic properties of 6-methyl-2-oxo-4-aryl-1,2,3,4-tetrahydropyrimidine-5-carboxylic acid esters. *Chemistry & Chemical Technology*, 14(3), 277–283. https://doi.org/10.23939/chcht14.03.277

8. Kostiuk, R. R., Horak, Y., Velychkivska, N., Sobechko, I. B., Pyshna, D. B., & Dibrivnyi, V. (2023). Thermodynamic properties of 2-methyl-5-phenylfuran-3-carboxylic. *Chemistry, Technology and Application of Substances*, 6(1), 8–14. https://doi.org/10.23939/ctas2023.01.008

9. Sobechko, B., Dibrivnyi, V. M., & Gorak, Yu. I. (2022). Enthalpy of formation and combustion of 5-(4-nitrophenyl)furan-2-carbaldehyde and its 2-methyl and 2-oxomethyl derivatives in the condensed state. *Chemistry, Technology and Application of Substances*, 5(2), 30–36. https://doi.org/10.23939/ctas2022.02.030

10. Rossini F. D. *Experimental Thermochemistry*. Interscience Publishers. N. Y.; London, 1956. Vol. 2. P. 326.

11. Nickel, J., Gohlke, B.-O., Erehman, J., Banerjee, P., Rong, W. W., Goede, A., Dunkel, M., & Preissner, R. (2014). SuperPred: *Update on drug classification and target prediction. Nucleic Acids Research*, 42(W1). https://doi.org/10.1093/nar/gku477

12. *Biological and bioorganic chemistry: textbook: in 2 books. Book 1. Bioorganic chemistry* / B. S. Zimenkovskyi,

D. S. Shevchenko, Y. I. Horak, N. I. Tischenko, D. B. Pyshna, I. B. Sobechko

V. A. Muzychenko, I. V. Nizhenkovska, G. O. Raw; under the editorship B. S. Zimenkovsky, I. V. Nizhenkovskaya. 3rd ed. K.: VSV "Medicine", 2022. 272 p. (in Ukrainian)

13. http://www.codata.info/resources/databases/key1.html

14. Acree, W., & Chickos, J. S. (2016). Phase transition enthalpy measurements of organic and organometallic compounds. sublimation, vaporization and fusion enthalpies from 1880 to 2015. part 1. C1− C10. *Journal of Physical and Chemical Reference Data*, 45(3), 033101. https://doi.org/10.1063/1.4948363

15. Benson, S. W. (1965). III − bond energies. *Journal of Chemical Education*, 42(9), 502. https://doi.org/10.1021/ed042p502

16. Domalski, E. S., & Hearing, E. D. (1993). Estimation of the thermodynamic properties of C-H-N-O-S- halogen compounds at 298.15 K. *Journal of Physical and Chemical Reference Data*, 22(4), 805–1159. https://doi.org/10.1063/1.555927

17. Cohen, N. (1996). Revised Group additivity values for enthalpies of formation (at 298 K) of carbon – hydrogen and carbon – hydrogen – oxygen compounds. *Journal of Physical and Chemical Reference Data*, 25(6), 1411–1481. https://doi.org/10.1063/1.555988

18. Salmon, A., & Dalmazzone, D. (2007). Prediction of enthalpy of formation in the solid state (at 298.15K) using second-order group contributions Part 2: Carbon-hydrogen, carbon-hydrogen-oxygen, and carbon-hydrogen-nitrogen-oxygen compounds. *Journal of Physical and Chemical Reference Data*, 36(1), 19–58. https://doi.org/10.1063/1.2435401

Д. С. Шевченко[1], Ю. І. Горак[2], Н. І. Тищенко[3], Д. Б. Пишна[1], І. Б. Собечко[1]

[1] Національний університет "Львівська політехніка",
кафедра фізичної, аналітичної та загальної хімії

[2] Львівський національний університет ім. І. Франка,
кафедра органічної хімії

[3] Інститут проблем матеріалознавства ім. І. М. Францевича НАНУ,
відділ фізико-хімії і технології наноструктурної кераміки та нанокомпозитів

ТЕРМОДИНАМІЧНІ ВЛАСТИВОСТІ
3-(1,5-ДИФЕНІЛПІРОЛ-2-ІЛ)-ПРОПАНОВОЇ КИСЛОТИ

Із використанням прецизійного обладнання експериментально визначено ентальпії випаровування, плавлення та утворення у конденсованому стані 3-(1,5-дифенілпірол-2-іл)- пропанової кислоти. Виконано розрахунок ентальпії сублімації за 298 К та ентальпії утворення в газоподібному стані. Наведено порівняльний аналіз експериментально визначених значень з теоретично розрахованими за адитивними методами розрахунку.

Ключові слова: енергія згоряння; ентальпія згоряння; ентальпія утворення; ентальпія випаровування; ентальпія плавлення; 3-(1,5-дифенілпірол-2-іл)-пропанова кислота.