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THERMODYNAMIC PROPERTIES OF 2-METHYL-5-PHENYLFURAN-3-CARBOXYLIC ACID

The temperature dependence of the saturated vapor pressure and the combustion energy of 2-methyl-5-phenylfuran-3-carboxylic acid were determined by experimental methods. Based on the obtained data, the values of the enthalpies of combustion and formation in the condensed state were calculated. The enthalpy of sublimation was recalculated to 298 K. The additive Benson scheme is supplemented with new fragments for calculating the enthalpies of formation in the gaseous state. The possibility of using the Joback method to calculate the enthalpies of formation of aryl furans in the gaseous state is analyzed.

Key words: combustion energy; enthalpy of combustion; enthalpy of formation; enthalpy of sublimation; 2-methyl-5-phenylfuran-3-carboxylic acid.

Introduction

2-methyl-5-phenylfuran-3-carboxylic acid is a heterocyclic compound of the aryl furan series. Substances of this series are used in the synthesis of biologically active compounds with pharmacophore properties. Aryl furans are components of medicines [1], for the treatment of genetic and neurodegenerative diseases [2], and in antiretroviral therapy [3]. In addition, substances of this series are used as modifying agents in copolymerization [4] and in the synthesis of catalysts [5, 6]. Despite the wide range of applications of arylfuran compounds, their thermodynamic properties have not been fully investigated.

The values of enthalpies of combustion of substances ($\Delta_c H^0_{298}$) belong to the main thermochemical characteristics, as they contain information about the energy of internal and intermolecular interactions. Calculated on their basis, the values of enthalpies of formation ($\Delta_f H^0_{298}$) in the condensed and gaseous state serve as key values when conducting thermodynamic calculations of chemical processes that occur with the participation of individual substances.

The present study is a continuation of thermodynamic studies of biologically active arylfuran derivatives, the results of which were published in [7–11].

Purpose of the work – using the method of bomb calorimetry, determine the energy of combustion of 2-methyl-5-phenylfuran-3-carboxylic acid and calculate the enthalpies of combustion and formation in the condensed state.

Materials and research methods

The synthesis of 2-methyl-5-phenylfuran-3-carboxylic acid was carried out according to the scheme shown in Fig. 1.

The reaction of sodium ethyl acetoacetate (**1**) with phenacylbromide (**2**) yielded ethyl-2-acetyl-4-oxo-4-arylbutanone (**3**), which was cyclized with phosphorus pentoxide in benzene to form ethyl ester of 2-methyl-5-phenylfuran-3-carboxylic acid (**4**). By saponification of the synthesized ester (**4**), 2-methyl-5-phenylfuran-3-carboxylic acid (**5**) was obtained. The resulting colorless acid (**5**) was filtered and recrystallized several times from ethanol. For thermochemical studies, we used acid samples obta-

ined after different recrystallization quantity, namely, samples No. 1 and 2 were taken after four and five times of recrystallization, respectively.

Identification of *2-methyl-5-phenylfuran-3-carboxylic acid* was carried out by NMR spectroscopy. The ^{1}H NMR spectra were recorded on a Varian 600 (600 mHz) using DMSO-d6 solvent. Chemical shifts (δ, ppm) are given relative to the DMSO signal (2.50 ppm): ^{1}H NMR (600 MHz, DMSO) δ 2.65 (s, 3H, CH3), 7.16 (d, J = 3.3 Hz, 1H, fur), 7.31 (t, J = 8.1 Hz, 1H, C6H5), 7.55 (d, J = 8.0 Hz, 2H, C6H5), 7.81 (d, J = 8.0 Hz, 2H, C6H5), 11.09 (bs, COOH).
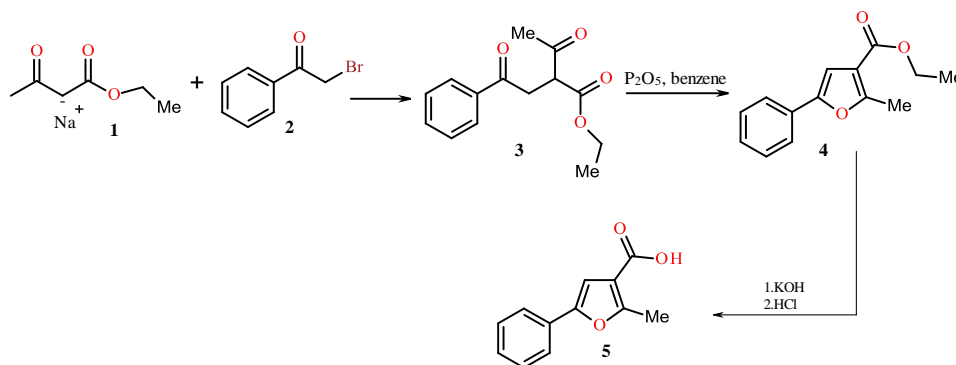

Fig. 1. Scheme of the synthesis of 2-methyl-5-phenylfuran-3-carboxylic acid

The enthalpy of acid sublimation was calculated from the temperature dependence of saturated vapor pressure determined by the Knudsen integral effusion method. The construction features of the effusion installation are similar to those described in [8]. The construction of the chamber and membranes is borrowed from [12]. The experimental methodology was selected according to the recommendations [12].

The vacuum system of the installation created a vacuum of 0,1 Pa in 45 ± 15s. The mass of the substance effused during the experiment (Δm_{ef}) was determined by the difference in the mass of the chamber before and after the experiment using the VLR-20 balance with an accuracy of $\pm 5 \cdot 10^{-6}$ g. The accuracy of maintaining the sample temperature (*T*) and the duration of the effusion (τ) was ± 0.1 K and ± 10s, respectively.

Reliability of the effusion installation was determined in many experiments to determine the temperature dependence of the vapor pressure of reference benzoic acid of grade K-1 in the temperature range of 322.7–353.5 K using a membrane with a thickness and diameter of 0.05 and 0.5903 mm. respectively. Volatile impurities that would distort the results of experimental studies were removed at the stage of surface formation of the test sample. This stage was considered complete when the sample effusion rate was reproduced within 1 % at a fixed temperature. The results of the experimental determi-

nation of the temperature dependence of the saturated vapor pressure of benzoic acid were processed by the least squares method and approximated as a linear equation: lnP(Pa) = (34.57 ± 0.96) – (11052 ± 326)1/T; correlation coefficient R = 0.997. The calculated value of the benzoic acid enthalpy of sublimation is 91,9 ± ± 1,1 kJ/mol. This value is in good agreement with the value of $\Delta_{sub}H = 93.0 \pm 4.0$ kJ/mol obtained by Ginkel and Kruif by the effusion method in the temperature range 294–331 K [13]. Hereinafter, the standard deviation of the average value is calculated without taking into account the Student's criterion.

The energy of combustion of 2-methyl-5-phenylfuran-3-carboxylic acid was determined using a precision combustion calorimeter B-08-MA with an isothermal shell (± 0.003 K) and a static calorimetric bomb. The energy equivalent of the calorimetric system (W = 15277 ± 8 J/V) was determined with an accuracy of ± 0.06 % under the conditions given in [11] by burning the reference benzoic acid of grade K-1 (a particularly pure compound with a mass fraction of the main substance of 99.995 % mol.).

The acid under study was in a solid aggregate state under normal conditions. Before the experiment, it was ground in a chalcedony mortar, tableted in a mold and placed in a platinum cup. The ignition of the samples under the experimental conditions was initiated by discharging capacitors through a nichrome wire, which set fire to a cotton thread. The initial pressure of oxygen, previously purified from

combustible impurities, carbon dioxide and water, was 30 atm. The temperature of the beginning of the main period in all experiments was 298.15 K.

After each combustion, the combustion products were quantitatively analyzed for the presence of mono- and dioxide, soot, and nitric acid. The amount of carbon dioxide formed was determined by the Rossini method [14] with an accuracy of $\pm 2 \cdot 10^{-4}$g. The reliability of gas analysis has been confirmed by many experiments on the combustion of reference benzoic acid. The carbon monoxide content was monitored in separate experiments using indicator tubes with an accuracy of $\pm 5 \cdot 10^{-6}$ g. The amount of soot formed on the walls of the platinum cup was determined by weighing with an accuracy of $\pm 5 \cdot 10^{-6}$ g.

The HNO_3 content was determined by titration with 0,1 N KOH.

Results and discussion

Experiments to determine the saturated vapor pressure of the acid were carried out in the same way as for benzoic acid. The results of effusion measurements, including the saturated vapor pressure of the substance (P), the linear equation of the temperature dependence of the saturated vapor pressure in the coordinates of the Clapeyron-Clausius equation, are shown in Table. 1. Since the values of the linear equations in both samples coincided within the error limits, the averaged equation was used to determine the enthalpy of sublimation ($\Delta_{sub}H$) of the acid, Table 1.

Table 1

Results of effusion studies of 2-methyl-5-phenylfuran-3-carboxylic acid

2-Methyl-5-phenylfuran-3-carboxylic acid; (solid)									
Sample	T, K	τ, s	$\Delta m \cdot 10^3$,g	P, Pa	Sample	T, K	τ, s	$\Delta m \cdot 10^3$,g	P, Pa
1	391.6	5419	1.00	0.3233	2	393.9	3642	0.95	0.4583
	395.0	5412	1.45	0.4714		394.6	3616	0.85	0.4134
	397.5	5452	1.70	0.5503		404.5	3618	2.20	1.082
	401.0	5457	2.70	0.8771		410.0	2718	2.90	1.913
	404.1	3631	2.45	1.201		412.9	3610	5.05	2.516
	411.9	3618	4.10	2.036		413.8	3618	5.40	2.688
	415.9	3612	7.00	3.499		415.9	3624	6.50	3.238
$\ln P = (38.4 \pm 1,2) - (15477 \pm 503) \cdot 1/T$					$\ln P = (37,5 \pm 1,4) - (15124 \pm 549)\,1/T$				
$\ln P = (38.0 \pm 1,0) - (15336 \pm 392) \cdot 1/T; \Delta_{sub}H = 127.5 \pm 3.2$ kJ/mol									

Table 2

Results of experimental determination of the combustion energies of 2-methyl-5-phenylfuran-3-carboxylic acid

Sample	m_{comp}, g	ΔT, V	Q_{fuser}, J	Q_{HNO_3}, J	Q_{carb}, J	$-Q_{V(298)}$, J/g	$m_{CO_2}^{exp}$ $m_{CO_2}^{calc}$
1	0.18853	0.34943	81.2	4.1	31.3	28029	0.9985
	0.24916	0.46284	86.4	8.9	28.1	28109	0.9968
	0.17519	0.32635	74.5	1.8	11.3	28088	0.9956
	0.18220	0.33775	70.9	3.0	18.4	28015	0.9998
$\Delta Q_{V(298)} = -28060 \pm 22$ J/g							
2	0.21573	0.40112	76.4	1.2	13.9	28111	0.9965
	0.11586	0.22740	91.3	5.9	29.2	28082	0.9999
	0.16757	0.31205	86.3	2.4	14.3	28005	0.9995
	0.20002	0.37133	74.9	3.0	16.2	28053	0.9975
$\Delta Q_{V(298)} = -28062 \pm 22$ J/g							
$\Delta Q_{V(298)\text{mean}} = -28062 \pm 13$ J/g							

The combustion energy ($Q_{V(298)}$) under the experimental conditions was calculated according to equation 1:

$$-Q_{V(298)} = \frac{W \cdot \Delta T - Q_{fuser} - Q_{HNO_3} + Q_{carb}}{m_{comp}} \quad (1)$$

where W – energy equivalent of the calorimetric system; m_{comp} – mass of the substance that was burned during the experiment; Q_{fuser}, Q_{HNO3}, Q_{carb} – 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 – 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 ($m_{CO_2}^{calc}$).

Since the values of the combustion energies of the two samples coincided, the averaged value was used to calculate the standard enthalpy of combustion $\Delta_c H^o_{298}$.

The $\Delta_c H^o_{298}$ (kJ/mol) of the acid was calculated taking into account the Washburn correction π [11] and the correction for the expansion work ΔnRT. To calculate the standard enthalpy of formation $\Delta_f H^0_{298}$ in the condensed state by the combustion reaction, we used the formation energies (kJ/mol): CO_2(g) = = 393.51 ± 0.13; H_2O(l) = 285.830 ± 0.040; O_2(g) = 0 [15]. The energy of combustion and enthalpy properties of the acid are given in Table 3.

The enthalpy of sublimation of the acid was determined in the temperature range determined by the conditions of the experiment. To recalculate the enthalpy of sublimation from the mean temperature of the studied interval (T_{mean}) to 298 K, the values of the change in heat capacity ΔC_p at this phase transition are necessary. Due to the absence of experimentally determined values of ΔC_p, we used two theoretical calculation methods, namely the method of Chikos and Agri [16] (equation (2)) and the semi-empirical calculation method [17] (equation (3)).

$$\Delta_{sub} H_{298} = \Delta_{sub} H_{T_{mean}} +$$
$$+ 0.75 + 0.15 \cdot C_{p\ c} \cdot T_{mean} - 298 \quad (2)$$
$$\Delta_{sub} H_{298} = \Delta_{sub} H_{T_{mean}} +$$
$$+ 0.259 \pm 0.041 \cdot M \cdot T_{mean} - 298 \quad (3)$$

where $C_{p\ c}$ – is the heat capacity of a substance in a solid aggregate state at 298 K, calculated by group contributions, for the acid under study is 266.0 (J/mol·K); M – the molecular weight of the substance is equal to 216.2 (g/mol).

Table 3

Energy characteristics of combustion and formation (kJ/mol)
2-methyl-5-phenylfuran-3-carboxylic 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)
− 5679.0 ± 2,6	−4.7	−2.5	-5681.2 ± 2.6	−469.8 ± 2.6	−337.1 ± 5.5

The enthalpy of sublimation of the acid was determined in the temperature range determined by the conditions of the experiment. To recalculate the enthalpy of sublimation from the mean temperature of the studied interval (T_{mean}) to 298 K, the values of the change in heat capacity ΔC_p at this phase transition are necessary. Due to the absence of experimentally determined values of ΔC_p, we used two theoretical calculation methods, namely the method of Chikos and Agri [16] (equation (2)) and the semi-empirical calculation method [17] (equation (3)).

$$\Delta_{sub} H_{298} = \Delta_{sub} H_{T_{mean}} +$$
$$+ 0.75 + 0.15 \cdot C_{p\ c} \cdot T_{mean} - 298 \quad (4)$$

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

where $C_{p\ c}$ – is the heat capacity of a substance in a solid aggregate state at 298 K, calculated by group contributions, for the acid under study is 266.0 (J/mol·K); M – the molecular weight of the substance is equal to 216.2 (g/mol).

The value of the enthalpy of sublimation of 2-methyl-5-phenylfuran-3-carboxylic acid at 298 K, calculated by equation (2), is 132.2 ± 3.8 kJ/mol, and by equation (3) 133.3 ± 3.1 kJ/mol. The results of the recalculation are in good agreement with each other, so the average value of the enthalpy of subli-

mation calculated by the two methods was used to calculate the enthalpy of acid formation in the gas phase. The value of the enthalpy of acid formation in the gaseous state, calculated taking into account the enthalpy of sublimation at 298 K, is given in Table 3.

The previously described procedure for the experimental determination of thermodynamic parameters is multistage and costly. Therefore, there is a need to use alternative methods for calculating thermodynamic parameters in the gas phase. Such methods include a number of additive calculation methods, of which the most popular are the Benson [18] and Joback [19] methods. These methods are based on the observation that most properties of rather complex molecules can be represented as the sum of the respective contributions of individual atoms or bonds. The forces that act between atoms within molecules or between atoms of different mo-
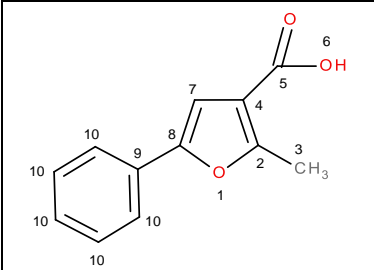
lecules are very close. Such individual atoms in any molecule make almost constant contributions to the ultraviolet and infrared absorption spectra, entropy, heat capacity, and heat of formation.

Therefore, the Benson method and the Joback method were chosen to calculate the enthalpies of formation of the studied substances in the gaseous state. Table 4 shows the group contributions required to calculate the enthalpy of formation in the gas phase by the Benson method.

The analysis of the test substance revealed the absence of three group contributions: C_d–$(C_d)(C_b)(O)$, C_d–$(C_d)_2(CO)$ and C–$(C_d)(H)_3$. The group contribution C_d–$(C_d)_2(CO)$ can be calculated on the basis of experimentally obtained values $\Delta_f H^o_{298}$ g 3-furancarbaldehyde and 3-furancarboxylic acid, and the contribution of C–$(C_d)(H)_3$ from $\Delta_f H^o_{298}$ g 2-methylfuran and 2,5-dimethylfuran, Table 5.
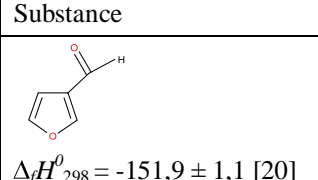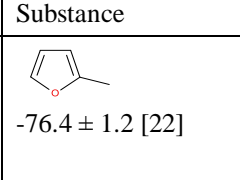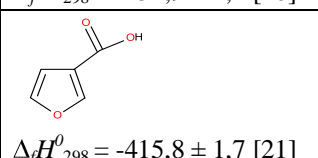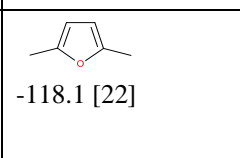
Table 4

Group contributions for the calculation of standard enthalpies of formation in the gaseous state at 298 K, (kJ/mol)

	No. group	Group	$\Delta_f H^0_{298}$	No. group	Group	$\Delta_f H^0_{298}$
	1	O–$(C_d)_2$	-137.2	7	C_d–$(C_d)(H)_2$	26.20
	2	C_d–$(C_d)(C)(O)$	43.1	8	C_d–$(C_d)(C_b)(O)$	***61.8***
	3	C–$(C_d)(H)_3$	***-49.2***	9	C_b–$(C_b)_2(C_d)$	23.8
	4	C_d–$(C_d)_2(CO)$	***41.4***	10	C_b–$(C_b)_2(H)$	13.8
	5	CO–$(C_d)(O)$	-140.2	Correction of furan cycle		-25.9
	6	O–(CO)(H)	-252.3			

*The values of group contributions, which were calculated using the substances studied in this work or substances taken from the literature, are highlighted in "**bold italics**".*

Table 5

Formation enthalpies of 3-furancarboxylic acid and 2-methylfuran derivatives and some group contributions kJ/mol

Substance	Group	$\Delta_f H^0_{298}$	Substance	Group	$\Delta_f H^0_{298}$
 $\Delta_f H^0_{298}$ = -151,9 ± 1,1 [20]	C_d–$(C_d)_2(CO)$	43.4	 -76.4 ± 1.2 [22]	C–$(C_d)(H)_3$	-49.1
 $\Delta_f H^0_{298}$ = -415,8 ± 1,7 [21]		39.4	 -118.1 [22]		-49.2
Mean value:		41.4		Mean value:	-49.2

The value of the group contribution of $C_d - (C_d)(C_b)(O)$ calculated from the acid under study is 62–1 kJ/mol, and from the ethyl ester of 2-cyano[3-(4-phenyl)-2-furan] acrylic acid $\Delta_f H_{298}^o \ g = -113.6 \pm \pm 7.1$ kJ/mol [7] is 61.4 kJ/mol. The mean value is 61.8 kJ/mol.

To verify the reliability of the determination of this group contribution, we calculated $\Delta_f H_{298}^o \ g$ of 2-methyl-5-(4-methylphenyl)-furan-3-carboxylic acid – 376.7 ± 5.9 kJ/mol [10] and ethyl ester of 2-cyano-3-[4-(4-methylphenyl)-2-furan] acrylic acid – 149.0 ± 8.5 kJ/mol [7]. The calculated values of $\Delta_f H_{298}^o \ g$ using the determined group contributions coincide within the errors of the experimentally determined values and are -370.4 and -145.9kJ/mol, respectively. Thus, the calculated values of the group contributions can be considered statistically reliable and can be used to calculate $\Delta_f H_{298}^o \ g$ of aryl furans.

Another, more modern and at the same time simple empirical method that allows us to estimate the thermodynamic properties of individual subs-tances is the Joback method [19]. This method is based on the principle that aspects of the structure of chemical components are always the same in many different molecules. Joback assumes that there is no interaction between groups, so it uses only additive contributions, without taking into account the immediate environment, and no contributions (corrections) to account for interactions between groups. This versatility of the method is considered an advantage, since a small number of standard group contributions and Equation 4 are required to calculate the thermodynamic parameters of complex substances.

$$\Delta_f H_{298}^o = 68.29 + \ H_{form}. \qquad (6)$$

Group contributions of formation enthalpies (H_{form}) according to the Joback method [19], which are necessary for the description of 2-methyl-5-phenylfuran-3-carboxylic acid (kJ/mol): (– CH_3 – 76.45); ((– O –)$_c$ – 138.16); (–COOH – 426.72); ((= CH –)$_c$ 2.09); ((= C <)$_c$ 46.34).

The calculated value of $\Delta_f H_{298}^o(g)$ of 2-methyl-5-phenylfuran-3-carboxylic acid is – 373.8 kJ/mol. The difference of 36.8 kJ/mol is significant, so it was decided to perform this calculation for other substances containing an arylfuran fragment. Thus, for 2-methyl-5-(4-methylphenyl)-furan-3-car-boxylic acid – 376.7 ± 5.9 kJ/mol, the calculated

value is – 404.9 kJ/mol for the ethyl ester of 2-cyano-3-[4-(4-methylphenyl)-2-furan] acrylic acid, the difference is 21.7 kJ/mol and for the ethyl ester of 2-cyano[3-(4-phenyl)-2-furan] acrylic acid – 26.0 kJ/mol. Thus, it is not entirely correct to consider the Joback method acceptable for estimating $\Delta_f H_{298}^o(g)$ of the class of substances under study.

Conclusion

As a result of the conducted research, the enthalpies of combustion (– 5681.2 ± 2.6 kJ/mol) and formation in the condensed state (– 469.8 ± ± 2.6 kJ/mol) of 2-methyl-5-phenylfuran-3-carbo-xylic acid were determined experimentally. The sublimation enthalpy (127.5 ± 3.2 kJ/mol) in the temperature range (391.6 – 415.9) was calculated based on the temperature dependence of the satu-rated vapor pressure. The listed value of the enthalpy of sublimation up to 298 K was used to calculate the enthalpy of formation in the gaseous state (–337.1 ± ± 5.5 kJ/mol). Benson's additive scheme was supplemented with new fragments ($C_d - (C_d)(C_b)(O)$, $C_d - (C_d)_2(CO)$ and $C - (C_d)(H)_3$) for calculating the enthalpies of formation in gaseous condition Large discrepancies (from 21.7 to 36.8 kJ/mol) between the experimentally obtained and calculated values of enthalpies of formation in the gaseous state using Jobak's method indicate the incorrectness of this method for estimating the enthalpies of formation of structurally complex substances.

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ТЕРМОДИНАМІЧНІ ВЛАСТИВОСТІ 2-МЕТИЛ-5-ФЕНІЛФУРАН-3-КАРБОНОВОЇ КИСЛОТИ

Експериментальними методами визначено температурну залежність тиску насиченої та енергію згорання 2-метил-5-фенілфуран-3-карбонової кислоти. На основі отриманих даних розраховано величини ентальпій згорання та утворення в конденсованому стані. Проведено перерахунок ентальпії сублімації до 298 К. Поповнено адитивну схему Бенсона новими фрагментами для розрахунку ентальпій утворення у газоподібному стані. Проаналізовано можливість застосування метода Джобака для розрахунку ентальпій утворення арилфуранів у газоподібному стані.

Ключові слова: енергія згорання; ентальпія згорання; ентальпія утворення; ентальпія сублімації; 2-метил-5-фенілфуран-3-карбонова кислота.