

THERMODYNAMIC PROPERTIES OF 6-METHYL-2-OXO-4-ARYL-1,2,3,4-TETRAHYDROPYRIMIDINE-5-CARBOXYLIC ACID ESTERS

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Abstract. Combustion energies of esters (ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate; ethyl 6-methyl-4-(4-methylphenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate; ethyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate and ethyl 4-(6-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate) were experimentally obtained using a bomb calorimetry. According to the experimental data, the enthalpies of combustion and the enthalpies of formation in a solid state were calculated. Derivative analysis was used to investigate the compounds within the temperature range of 483.0–577.5 K. The enthalpies of fusion, vaporization and sublimation were calculated using the results of the differential thermal analysis. According to the obtained data, the enthalpies of formation of the investigated compounds in the gaseous state were calculated. The possibility of using the Benson additive scheme to calculate the enthalpy of formation is demonstrated.

Keywords: enthalpy of combustion, enthalpy of formation, enthalpy of fusion, enthalpy of vaporization, enthalpy of sublimation, 6-methyl-2-oxo-4-aryl-1,2,3,4-tetrahydropyrimidine-5-carboxylic acid esters.

1. Introduction

A great number of modern drugs has been formed on the basis of five-membered heterocycle compounds with one or two heteroatoms. The application of mentioned compounds became possible due to the biological activity of natural heterocyclic compounds. Diverse study of their synthetic analogues would contribute to the creation of drugs of new generation.

Among them esters of 6-methyl-2-oxo-4-aryl-1,2,3,4-tetrahydropyrimidine-5-carboxylic acids (DHPM) are of great interest. These biologically active compounds are used for the production of drugs with different pharmaceutical properties, in particular anti-microbial properties, and for the production of drugs preventing neurodegenerative and oncological diseases.

The current interest of researchers and pharmacologists in DHPM esters is associated primarily with the fact that adrenergic receptor antagonists are useful for the treatment of benign prostatic hyperplasia [1]. Interesting biological effects have also been identified for DHPM analogue as a potential new antitumor agent which is involved in blocking mitosis by inhibiting kinesin motor protein, which is just one example [2]. It was also found [3] that some natural compounds that exhibit strong selective activity against HIV-1 have a fragment of dihydropyrimidines. Thus, it can be said that these compounds have a wide range of biological activity [4].

Based on the above mentioned, it can be stated with certainty that the rapid development of these compounds synthesis is due to the prospect of their use in medicine and pharmaceuticals [5, 6]. Therefore, the study of their thermodynamic parameters is important for determining the reaction energies of the synthesis and for understanding the mechanisms of reactions involving them, as well as for calculating the chemical equilibrium in processes involving mentioned compounds.

The synthesis of drugs is mostly carried out in a medium of solvent using the reactants of pure analytical grade. The purity of the substances is ensured by repeated purification processes which include distillation, sublimation and recrystallization. The latter process is carried out using widely used solvents. Therefore, the study of solubility and thermodynamic parameters that accompany the process of solvent interaction with a solute, would allow to optimize the synthesis processes and purification of organic compounds.

This work is a continuation of a series of our studies related to the determination of thermodynamic parameters of individual organic compounds and their solutions [7-10].

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2. Experimental

The synthesis of esters was carried out at the Department of Organic Chemistry at Ivan Franko National University of Lviv according to the procedure described in [11]. The synthesis was carried out in a glass reactor loaded with corresponding aromatic aldehyde, urea, methyl or ethyl esters of acetoacetic acid in the presence of concentrated hydrochloric acid, in the medium of ethanol. The mixture was boiled for 3 h, then it was cooled to 273 K and left to crystallize. The obtained precipitate was filtrated and then purified by double recrystallization from ethanol.

The compounds purity was determined by chromatography using an Agilent 1100 HPLC equipped with a diode matrix and a mass selector on a Zorbax SB-C18 column (4.6×15 mm); eluent was A acetonitrile-water with 0.1% TFA.

The structural formulas and purity of the investigated compounds are shown in Table 1.

The synthesized esters were identified by NMR spectroscopy using Varian 400 (400 MHz) and DMSO-D₆ solvent. The chemical shifts (δ , ppm) recorded relatively to DMSO signal (2.5 ppm) are also shown in Table 1. The combustion energy of the compounds was determined on a precision calorimeter B-08-MA with an isothermal shell (± 0.003 K) and a static calorimetric bomb. The energy equivalent of the calorimetric system was determined with the accuracy of $\pm 0.06\%$ by the combustion of the reference benzoic acid of K-1 brand (main component content is 99.995 ± 0.01 mol %). The heat of combustion of benzoic acid, taking into account the Jessup factor is $\Delta U_B = -26434.4$ J/g. The combustion was carried out at 298 K in an oxygen atmosphere at a pressure of $3.04 \cdot 10^6$ Pa. Hereinafter, the standard deviation of the mean values is calculated using the Student's criterion for a 5% significance level.

Table 1

The structural formulas and purity of 6-methyl-2-oxo-4-aryl-1,2,3,4-tetrahydropyrimidine-5-carboxylic acids esters

Symbol	Compound	Structural formula	Chemical shifts	Content of main compound, wt %
I	Ethyl 6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate C ₁₃ H ₁₄ N ₂ O ₃		¹ H NMR δ : 1.09 (t, J 8,0, 3H, CH ₃ CH ₂), 2.25 (s, 3H, CH ₃), 3.97 (q, J = 8.0 Hz, 2H, CH ₂), 5.14 (s, 1H, CH), 7.20–7.36 (m, 5H, Ph), 7.74 (s, 1H, NH), 9.19 (s, 1H, NH)	99.9
II	Ethyl 6-methyl-4-(4-methylphenyl)-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate C ₁₄ H ₁₆ N ₂ O ₃		¹ H NMR (400 MHz, DMSO) δ : 9.10 (s, 1H, NH), 7.63 (s, 1H, NH), 7.07 (s, 4H C ₆ H ₄), 5.06 (s, 1H, CH), 3.95–3.90 (m, 2H, OCH ₂ CH ₃), 2.20 (s, 3H, CH ₃), 2.21 (s, 3H, CH ₃), 1.05 (t, J = 6.9 Hz, 3H, OCH ₂ CH ₃)	99.9
III	Ethyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate C ₁₄ H ₁₆ N ₂ O ₄		¹ H NMR (400 MHz, DMSO) δ : 9.09 (s, 1H, NH), 7.61 (s, 1H, NH), 7.09 (d, J = 8.3 Hz, 2H, C ₆ H ₄), 6.82 (d, J = 8.5 Hz, 1H, C ₆ H ₄), 5.04 (s, 1H, CH), 4.01–3.85 (m, 2H, OCH ₂ CH ₃), 3.68 (s, 3H, CH ₃ O), 2.20 (s, 3H, CH ₃), 1.06 (t, J = 6.9 Hz, 3H, OCH ₂ CH ₃).	99.8
IV	Ethyl 4-(6-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate C ₁₄ H ₁₆ N ₂ O ₄		¹ H NMR (400 MHz, DMSO) δ : 9.06 (s, 1H, NH), 7.27–7.14 (m, 2H, NH + C ₆ H ₄), 7.00 (d, J = 5.9 Hz, 1H, C ₆ H ₄), 6.94 (d, J = 7.7 Hz, 1H, C ₆ H ₄), 6.83 (d, J = 6.8 Hz, 1H, C ₆ H ₄), 5.45 (s, 1H, CH), 3.92–3.84 (m, 2H, OCH ₂ CH ₃), 3.75 (s, 3H, CH ₃ OC ₆ H ₄), 2.23 (s, 3H, CH ₃), 0.98 (t, J = 6.8 Hz, 3H, OCH ₂ CH ₃).	99.7

Under normal conditions the investigated compounds are solid. Before the experiments the samples were compressed into a tablet using a stainless steel press form and hand press.

The weight of the burned compound was determined according to the CO₂ amount in the gaseous combustion products with the accuracy of $\pm 1 \cdot 10^{-4}$ g. The amount of soot formed at the sides of platinum dish was determined by weighting the dish with the accuracy of $\pm 5 \cdot 10^{-6}$ g. The amount of HNO₃ formed in the experiment was determined by titration with 0.1N KOH solution [12].

The enthalpies of the phase transitions were calculated according to the data of derivatographic analysis, which was performed using two different Q-1500 D derivatographs of the Paulik-Paulik-Erdey system. Samples were analyzed in the corundum and platinum crucibles under dynamic mode with heating rates of 2.5 and 5 K/min [13].

Enthalpy of vaporization ($\Delta_{\text{vap}}H$) was determined by the temperature dependence of their vaporization rate $v = \Delta m / \Delta \tau$ in that temperature range where the compounds were in a liquid state prior to the beginning of the degradation processes. The integral curve of weight loss was differentiated every 30 seconds. The temperature dependences of the evaporation rate of the compounds were analyzed in the coordinates of the Arrhenius equation $\ln v = A - B/T$, where $B = E_{\text{act}}/R$. Condensation of vapor in the presence of a liquid phase is an activationless process, so it can be assumed that the enthalpy of activation of this process and $\Delta_{\text{vap}}H$ are equal (Eq. 1)

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

The enthalpy of fusion ($\Delta_{\text{fus}}H$) was calculated taking into account the heat absorbed by vaporization of the lost mass of the sample (Eq. 2).

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

where Q_{fus} and Q_{vap} are the amount of heat absorbed during fusion or evaporation of the sample, respectively, J; m_0 is the mass of the sample corresponding to the temperature of its fusion beginning T_{fus} , g; Δm_{vap} is the weight loss of the sample (vapor mass) over the period taken into account when determining the peak area S (K·s) under the DTA curve, g; K is a heat transfer coefficient, determined individually for applied derivatographs, using samples of adipic acid, biphenyl, silver nitrate and reference benzoic acid K-1, J/(K·s), $\Delta_{\text{fus}}H$ and $\Delta_{\text{vap}}H$ are specific enthalpies of fusion and vaporization of the compound, respectively, J/g.

3. Results and Discussion

The values of heat of combustion and combustion completeness of the compounds determined by the calorimetric method are given in Table 2.

The values of the standard enthalpy of combustion $\Delta_c H^0_{298}$ (kJ/mol) of the investigated compounds were calculated by the average values of internal energy change under the experimental conditions, taking into account the Washburn correction π [14] and the correction for expansion energy ΔnRT .

The standard formation enthalpies $\Delta_f H^0_{298}$ of the investigated compounds were calculated using standard enthalpy of combustion and standard formation enthalpy of combustion products [15].

The results of the calorimetric determination of standard enthalpies of combustion and formation of investigated compounds in the solid state at 298 K are shown in Table 3.

The parameters of the vaporization determined by derivatography are represented in Table 4.

The values of the enthalpy of fusion ($\Delta_{\text{fus}}H$) calculated by Eq. (2) are given in Table 5.

The values of enthalpy of sublimation ($\Delta_{\text{sub}}H$, Table 6), required to calculate the enthalpy of formation in the gaseous state, were calculated according to Eq. (3):

$$\Delta_{\text{sub}}H = \Delta_{\text{fus}}H + \Delta_{\text{vap}}H \quad (3)$$

These values were calculated at fusion points of the compounds, and the enthalpies of the formation in the condensed state – at 298 K. The values of phase transitions enthalpy are recalculated according to the Kirchhoff equation in which the change in heat capacity ΔC_p during the corresponding phase transition is unknown and determined experimentally. In the absence of experimentally determined values ΔC_p , we used two known methods of calculation:

i) the method of additive group contributions of Chikos and Agri [16], in which the values of the heat capacity of compounds in the solid state are calculated by the additive scheme;

$$\Delta_{\text{sub}}H_{298.15} = \Delta_{\text{sub}}H_{T_{\text{fus}}} + (0.75 + 0.15 \cdot \text{solid}C_{p298.15}) \cdot (T_{\text{fus}} - 298.15) \quad (4)$$

ii) the semi-empirical method of calculation [16];

$$\Delta_{\text{sub}}H_{298.15} = \Delta_{\text{sub}}H_{T_{\text{fus}}} + (0.259 \pm 0.041) \cdot M \cdot (T_{\text{fus}} - 298.15) \quad (5)$$

The results of the recalculations are given in Table 6.

The calculated values of enthalpy of sublimation differ from each other within the error of the experiment, indicating that both methods can be used for the calculations.

With the help of the obtained values we were able to calculate the enthalpies of the formation for the investigated compounds in the gas phase. Many previous publications [17, 18] proved the effectiveness of using the Benson additive scheme for the calculation of enthalpy of compound formation relative to group contributions. Therefore, we decided to test the possibility of applying this scheme to the compounds under study. The values necessary for the calculations are given in Table 7 [19].

Table 2

Heat of combustion of the compounds in a solid state

Compound symbol	Synthesis number*	<i>m</i> , g	ΔT , V	$-\Delta_c U$, J·g ⁻¹	$m_{\text{exp}}/m_{\text{calc}}$
I	1	0.24486	0.66014	27592	0.9996
	1	0.12809	0.34956	27647	0.9999
	1	0.19232	0.52204	27643	0.9979
	1	0.23127	0.62511	27597	0.9985
	2	0.23505	0.63590	27616	0.9996
	2	0.30622	0.82599	27651	0.9989
	2	0.36359	0.97742	27617	0.9969
	2	0.39177	1.05437	27638	0.9976
Average value $-\Delta_c U = 27625 \pm 19$					
II	1	0.33538	0.93305	28533	0.9975
	1	0.27051	0.75193	28544	0.9999
	1	0.19350	0.54012	28559	0.9986
	1	0.12560	0.35352	28566	0.9989
	2	0.26179	0.72896	28559	0.9995
	2	0.21739	0.60837	28551	0.9993
	2	0.33475	0.93308	28571	0.9986
	2	0.12171	0.34390	28567	0.9979
Average value $-\Delta_c U = 28556 \pm 12$					
III	1	0.15508	0.40343	26510	0.9989
	1	0.26073	0.67660	26533	0.9996
	1	0.10943	0.28879	26568	0.9990
	1	0.09685	0.25633	26539	0.9976
	2	0.19358	0.50419	26544	0.9999
	2	0.34368	0.88743	26518	0.9989
	2	0.33436	0.86348	26532	0.9980
	2	0.26621	0.68978	26568	0.9986
Average value $-\Delta_c U = 26539 \pm 17$					
IV	1	0.14044	0.36578	26485	0.9998
	1	0.13356	0.34743	26493	0.9986
	1	0.10903	0.28530	26512	0.9999
	1	0.16190	0.42091	26509	0.9985
	2	0.17948	0.46091	26521	0.9990
	2	0.35435	0.91499	26475	0.9979
	2	0.31425	0.81070	26501	0.9986
	2	0.31793	0.82084	26507	0.9991
Average value $-\Delta_c U = 26500 \pm 16$					

Note: * the compounds obtained during two different syntheses were used

Table 3

Energy, standard enthalpy of combustion and formation enthalpy of investigated compounds in a solid state, kJ/mol

Compound symbol	$-\Delta_c U$	$-\pi$	$-\Delta nRT$	$-\Delta_c H_{298}^0$	$-\Delta_f H_{298}^0$
I	7195.4 ± 4.9	4.9	3.7	7199.2 ± 4.9	596.6 ± 6.3
II	7838.6 ± 3.4	5.1	5.0	7843.6 ± 3.4	631.6 ± 3.4
III	7710.1 ± 5.1	5.3	3.7	7713.8 ± 5.1	761.4 ± 5.1
IV	7698.9 ± 4.6	5.3	3.7	7702.6 ± 4.6	772.6 ± 4.6

Table 4

Parameters of vaporization process according to DTA

Compound symbol	Synthesis number	Temperature range, K	$\Sigma\Delta m' \cdot 10^3$, g	A	-B	$\Delta_{vap}H$, kJ/mol
I	1	512.8–564.8	2.94	18.32	11091	96.2
	1	529.2–578.7	8.41	18.15	10832	94.0
	2	489.7–553.3	15.7	20.01	11014	95.6
	2*	498.4–533.0	1.59	18.78	10846	94.2
	Average value $\Delta_{vap}H = 95.0 \pm 1.7$					
II	1*	549.8–579.9	1.78	22.31	13347	115.1
	2*	528.8–556.9	1.01	23.22	13017	112.3
	Average value $\Delta_{vap}H = 113.7 \pm 4.4$					
III	1	505.5–549.6	0.81	23.59	14381	123.6
	2	525.5–534.6	0.30	23.38	14238	123.4
	2*	543.3–576.1	1.35	23.74	14600	125.4
	Average value $\Delta_{vap}H = 123.8 \pm 2.8$					
IV	1	543.5–569.0	6.52	27.38	16473	141.4
	1*	550.6–586.7	2.03	28.72	16403	140.8
	2	549.4–566.5	10.3	26.76	16225	139.3
	2*	547.7–582.2	3.27	29.47	16581	142.3
	Average value $\Delta_{vap}H = 141.0 \pm 2.0$					

Note: * platinum crucible, heating rate is 5 K/min

Table 5

Enthalpies of fusion of the investigated compounds at the fusion point

Compound symbol	Synthesis number	m_0 , g	Δm_{vap} , g	S, K·s	K, J/K·s	q_{vap} , J	$\Delta_{fus}H$, kJ/mol
I $T_{fus} = 480.6 \pm 1.1$ K	1	0.2014	0.0013	737.4	0.04536	0.4883	42.6
	1	0.1985	0.0022	765.0	0.04536	0.8078	44.4
	2	0.2040	0.0052	823.5	0.04536	1.906	45.2
	2	0.1034	0.0003	406.7	0.04271	0.1218	43.4
	Average value $\Delta_{fus}H = 43.9 \pm 1.8$						
II $T_{fus} = 494.4 \pm 1.0$ K	1	0.0544	0.0002	222.5	0.04394	0.0814	48.9
	2	0.0175	0.0004	75.9	0.04394	0.1602	49.9
	Average value $\Delta_{fus}H = 49.4 \pm 1.6$						
III $T_{fus} = 481.3 \pm 1.1$ K	1	0.2017	0.0002	685.9	0.04547	0.0947	44.5
	2	0.2000	0.0005	666.7	0.04547	0.2270	43.7
	2*	0.1037	0.0002	373.5	0.04277	0.0908	44.7
	Average value $\Delta_{fus}H = 44.3 \pm 1.0$						
IV $T_{fus} = 534.4 \pm 1.8$ K	1	0.1982	0.0091	876.0	0.05416	4.397	63.1
	1	0.1047	0.0020	511.7	0.04749	0.9891	64.7
	2	0.1981	0.0178	981.1	0.05416	8.656	65.2
	2	0.0190	0.0009	96.5	0.4749	0.4364	63.5
	Average value $\Delta_{fus}H = 64.1 \pm 1.6$						

Note: * platinum crucible, heating rate is 5 K/min

Table 6

Enthalpy of sublimation of the investigated compounds, kJ/mol

Compound symbol	T_{fus} , K	$\Delta_{sub}H_{T_{fus}}$	$\Delta_{sub}H_{298}$ according to Eq. (4)	$\Delta_{sub}H_{298}$ according to Eq. (5)
I	480.6 ± 1.1	138.9 ± 2.5	148.5 ± 3.0	151.2 ± 2.9
II	494.4 ± 1.0	163.1 ± 4.7	174.3 ± 5.2	177.1 ± 5.4
III	481.3 ± 1.1	168.1 ± 3.0	183.6 ± 3.5	187.0 ± 3.4
IV	534.4 ± 1.8	205.1 ± 2.6	218.6 ± 3.1	222.9 ± 3.0

The experimental and calculated according to the Benson additive scheme values of the enthalpy of formation of the investigated compounds in the gas phase are represented in Table 8. For the compound I, the enthalpy of formation the calculated value practically coincides with the experimentally determined one. For compounds II and III, having a substituent at the benzene ring in the *para*-position, a deviation of 26.5 ± 2.5 kJ/mol is observed, which can be explained by the additional

interaction of this substituent with the methyl-oxo(CH₃O–) group. The most interesting results were obtained for the compound IV having a methyl-oxo substituent at the benzene ring in the *ortho*-position. The deviation from the Benson scheme for this compound is 53.1 kJ/mol, which can be explained by the interaction of oxygen of the methyl-oxo group and hydrogen bonded to nitrogen in the heterocycle, as well as by the formation of an intramolecular hydrogen bond.

Table 7

Group contributions necessary to calculate the enthalpy of formation of investigated compounds in the gas state (kJ/mol)

Increment	$\Delta_f H_{298}^0$	Increment	$\Delta_f H_{298}^0$
C – (C) (H) ₃ ≡ C – (C _b) (H) ₃ ≡	-42.2	O – (C _b) (C)	-94.6
C – (C _d) (H) ₃ ≡ C – (O) (H) ₃		O – (C) (CO)	-172.8
N – (C _d) (CO) (H)≡ N – (C) (CO) (H)	-18.4	C _b – (C _b) ₂ (C)	23.0
C – (C) (O) (H) ₂	-35.6	C _b – (C _b) ₂ (H)	18.3
C – (C _d) (C _b) (N) (H)	-21.8	C _b – (C _b) ₂ (O)	-7.5
C _d – (C _d) (C) (N)	45.2	CO – (C _d) (O)	-140.2
C _d – (C) (CO)	39.3	CO – (N) ₂	-131.8

Table 8

Enthalpies of formation of the investigated compounds in the gas phase (kJ/mol)

Compound symbol	$-\Delta_f H_{298}^0, \text{ g}$		Δ
	experimental	calculated	
I	446.7 ± 7.6	446.9	0.2
II	455.9 ± 8.2	479.9	24.0
III	576.1 ± 7.1	605.0	28.9
IV	551.9 ± 6.3	597.6	53.1

4. Conclusions

The enthalpies of combustion, formation, fusion, vaporization and sublimation of 6-methyl-2-oxo-4-aryl-1,2,3,4-tetrahydropyrimidine-5-carboxylic acids were determined. The possible use of the Benson additive scheme for this class of compounds was demonstrated. The obtained experimental and calculated data may be used to predict the reactivity of the investigated compounds, to calculate the energy parameters of the processes they are involved in, as well as to optimize their synthesis and purification processes.

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ТЕРМОДИНАМІЧНІ ВЛАСТИВОСТІ ЕСТЕРІВ 6-МЕТИЛ-2-ОКСО-4-АРИЛ-1,2,3,4-ТЕТРАГІДРОПРИМІДИН-5-КАРБОНОВИХ КИСЛОТ

Анотація. *Методом бомбової калориметрії експериментально одержані енергії згоряння естерів: етил 6-метил-2-оксо-4-феніл-1,2,3,4-тетрагідропіримідин-5-карбоксилат; етил 6-метил-4-(4-метилфеніл)-2-оксо-1,2,3,4-тетрагідропі-*

римідин-5-карбоксилат; етил 4-(4-метоксифеніл)-6-метил-2-оксо-1,2,3,4-тетрагідропіримідин-5-карбоксилат; етил 4-(2-метоксифеніл)-6-метил-2-оксо-1,2,3,4-тетрагідропіримідин-5-карбоксилат. За експериментальними даними розраховані ентальпії згоряння та ентальпії утворення в твердому стані. Дериватографічним методом проведено аналіз досліджених речовин в діапазоні температур 483,0–577,5 К. За даними диференційно-термічного аналізу розраховано величини ентальпій плавлення, випаровування та сублімації. За одержаними даними розраховані ентальпії утворення досліджених речовин в газоподібному стані. Продемонстровано можливість використання адитивної схеми Бенсона для розрахунку ентальпії утворення.

Ключові слова: *ентальпія згоряння, ентальпія утворення, ентальпія плавлення, ентальпія випаровування, ентальпія сублімації, естери 6-метил-2-оксо-4-арил-1,2,3,4-тетрагідропіримідин-5-карбонових кислот.*