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THERMOCHEMISTRY OF ANTICANCER ACTIVE MOLECULES: ENTHALPIES OF SOLUTION, SOLVATION, AND SUBLIMATION/VAPORIZATION FOR PHENYL ACETATE AND PARA SUBSTITUTED PHENYL BENZOATE COMPOUNDS

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ABSTRACT. The solution, solvation, and evaporation enthalpies of phenyl esters indicate the stability and quality of the molecules. Therefore, the phase-transition enthalpies of the phenyl esters evaluate molecular activity, efficiency, and stability. In this work, solution, solvation, and sublimation/vaporization enthalpies for para-substituted phenyl esters were determined using adiabatic solution calorimetry at 298.15 K. For the first time, the solution enthalpy of the phenyl esters was determined in benzene. The enthalpy of solvation was estimated using an additive scheme approach, the Abraham model, molar refraction, and solution calorimetry at standard temperature. In addition, we predicted solvation enthalpy values for the ethyl, propyl, and butyl groups in the phenyl ester compounds for the first time. Additionally, the solution and evaporation enthalpy measurements had the lowest standard deviations. Moreover, the values of evaporation enthalpy of the compounds in this work were discussed in comparison with those literature data.

KEY WORDS: Evaporation enthalpy, Solvation enthalpy, Solution calorimetry, Phenyl Ester

INTRODUCTION

Because of their vital medical uses, enthalpies of solution, solvation, and sublimation/vaporization of organic molecules have been studied. Aromatic organic compounds are commonly employed in medicine to make medications for conditions including cancer. Numerous attempts have been made in recent years to treat different types of cancer. Likewise, medications are created with compounds like phenyl benzoate and phenyl ester complexes that have been shown to have anticancer properties. As ligands for central metallic atoms like copper, phenyl esters are used. Additionally, the phenyl esters are used as inhibitors in anticancer instances [1-3].

Considering this, the molecular study proposes that determining a drug's anticancer effectiveness should be the initial step in creating treatments for cancer and depression. Phase transition thermodynamics, of course, demonstrates the medications' stability and quality. Even more important is the capacity to examine the thermochemistry of such substances. Moreover, the enthalpies of solvation and evaporation of the organic aromatic molecules have a special impact when used correctly. Further, Michael H. Abraham and William E. Acree and his colleagues assessed the theoretical methods in determining the solvation enthalpy for organic compounds using atomic data characteristics for solutes and solvents [4]. In addition, in a more straightforward manner, Professor Solomonov and his colleagues presented an innovative method for solvation enthalpy estimation for organic aromatic and heteroaromatic compounds in a variety of solvents, including acetonitrile and benzene. This methodology is known as the additive scheme approach [5], it was applied in studying many organic aromatic compounds [6, 7]. Moreover, there are two other methods in estimation enthalpy of solvation compounds except the two main methods mentioned above, there are the solution calorimetry-additivity scheme approach and the molar refraction method.

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Another property of phase transition thermodynamic parameters is the enthalpy of evaporation (enthalpy of sublimation/vaporization) of the compounds. There are many methods to determine the enthalpy of evaporation for organic and inorganic compounds [8]. In the previous works, it has been studied on determination of enthalpy of sublimation/vaporization of the organic aromatic compounds through applying various methods like solution calorimetry-additive scheme method, transpiration method [9] and correlation gas chromatography method [6, 10].
Correspondingly, the enthalpy of sublimation/vaporization of organic aromatic compounds was estimated from the solution calorimetry-additivity scheme approach at 298.15 K, according to the following Equation:

$$\Delta^{g}_{cr,liq}H^{Ai}_{m}(298.15\ K) = \Delta_{soln}H^{Ai/S}_{m}(298.15\ K) - \Delta_{solv}H^{Ai/S}_{m}(298.15\ K) \quad (1)$$

Where $\Delta^{g}_{cr,liq}H^{Ai}_{m}$ is the standard molar enthalpy of evaporation (sublimation/vaporization) for *Ai* compound as crystalline or liquid state, $\Delta_{soln}H^{Ai/S}_{m}(298.15\ K)$ is the molar enthalpy of solution compound *Ai* in solvent *S* at 298.15 K and $\Delta_{solv}H^{Ai/S}(298.15\ K)$ is the solvation enthalpy of the compound *Ai* to solvent *S* at 298.15 K [11].

In the present study aimed applying the solution calorimetry at 298.15 K, the enthalpies of solution, solvation, and evaporation are determined for compounds containing methyl para substituted benzoates and phenyl acetate in the current study (Figure 1). Next, the enthalpy of solution in benzene solvent was determined for the compounds at standard temperature. Additionally, the solution calorimetry-additive scheme approach was used for estimating the enthalpies of solvation and evaporation. Further, in a unique step, the enthalpy of solvation was calculated for alkyl-attached groups. Furthermore, information from publications was gathered to figure out and comparing the enthalpy of sublimation/vaporization for parasubstituted compounds containing ethyl, propyl, and butyl benzoate. Moreover, the Abraham model, molar refraction, solution calorimetry, and additive scheme were used to obtain the enthalpy of solvation values.

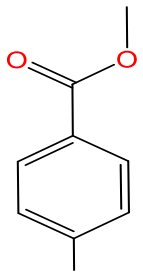


Figure 1. Chemical structure of a para-substituted phenyl ester.

EXPERIMENTAL

Materials

The components with high mass fraction purity were phenylacetate and derivatives of para-substituted phenyl ester, both of commercial provenance (Table 1). In this work, the purity percentage of all the compounds was equal to or higher than 97%. Benzene solvent was placed into the calorimetry Dewar cells. Prior to use them in the solution calorimetry technique, benzene solvent performed distillation and purification. Acetonitrile and benzene were fractionally distilled over P_2O_5 using conventional technique [12], and their mass purity fraction was further increased to 99.99%. The 7820 A gas chromatography method was used to establish the purities.
Table 1. CAS number, origin and mass purity of the phenyl esters.

Compound	CAS	Origin	Purity %
Methyl 4-fluorobenzoate	403-33-8	ACROSS ORGANICS	98
Methyl 4-chlorobenzoate	1126-46-1	Alfa Aesar	99
Methyl 4-bromobenzoate[a]	619-42-1		
Methyl 4-aminobenzoate	619-45-4	SIGMA ALDRICH	98
Phenyl acetate	122-79-2	ACROSS ORGANICS	97
Methyl benzoate[a]	93-58-3		
Methyl phenyl acetate[a]	101-41-7		
Ethyl benzoate[a]	93-89-0		
Ethyl 4-hydroxybenzoate[a]	120-47-8		
n-Propyl benzoate[a]	2315-68-6		
Propyl 4-hydroxybenzoate[a]	94-13-3		
n-Butyl benzoate[a]	136-60-7		

[a] Compounds were not practically worked on in the laboratory, therefore, their origin and purity percent were removed.

Solution calorimetry

The enthalpy of solution for the phenyl ester derivatives in acetonitrile/benzene solvents at 298.15 K was measured using the adiabatic solution calorimetry TAM III (TA Instruments, USA). The calorimeter works at a temperature stability of ± 0.01 K. The calorimeter's middle position was maintained for at least 30 minutes to establish thermal equilibrium; the technique works with continuous stirring at the start of the experiment. The chemicals used in this investigation were inserted into the solution calorimetry Dewar cell after being dissolved in a solvent. Based on their physical states, the examined compounds are separated into two groups: some are in the liquid form, and others are in the crystalline state.

For the crystalline compounds, first, the compounds were ground using a stone mortar. Then, about 0.5 mg of the sample was weighed and added to the ampoule cell, which was connected to the syringe and immersed in the glass cell of the calorimeter. On the other side, the liquid compounds were measured by adding to the glass cell of the calorimetry through a syringe in the range of 50- 100 µL of the liquid compound. The solution calorimetry procedure was described in more detail elsewhere [6, 13].

In the beginning, solution calorimetry was examined for two standards in distilled and deionized water solvents before measuring the enthalpy of solution of the phenyl ester compounds; the crystalline and liquid standard compounds were used separately. Potassium Chloride was used as a crystalline solid standard compound. The enthalpy of solution for KCl in deionized distilled water solvent was 17.48 ± 0.08 kJ/mol; it has excellent agreement with the literature value, which is 17.21 ± 0.09 kJ.mole^{-1} [14]. On the other hand, the high-purity 1-propanol compound was used as a liquid standard sample. The 1-propanol compound was dissolved in the purified water (distilled and deionized) and its enthalpy of solution was -10.16 ± 0.05 kJ.mole^{-1} it is well agree the value solution enthalpy in the literature -10.13 ± 0.09 kJ.mole^{-1} [15] for the same standard compound at 298.15 K.

RESULTS AND DISCUSSION

At normal temperature, multiple methods were utilized to figure out the enthalpies of solution, solvation, and evaporation. Solution calorimetry was applied to precisely determine the enthalpy of solution for the chemicals under study at absolute temperature. However, a number of approaches, such as solution calorimetry, the Abraham model, the additive scheme approach, and molar refraction, were utilized to predict the solvation enthalpy. Additionally, the solution calorimetry-additive scheme method has been employed to measure the enthalpy of

sublimation/vaporization. In a comparable way, data from the literature are compared with the measured values of the enthalpies.

Furthermore, the evaporation enthalpy reveals the chemical stability. The solubility of materials is represented by the solvation and solution enthalpies. As a result, the compounds' evaporation, solution, and solvation enthalpies in this study serve as indicators of the effectiveness and caliber of the molecules used to make the anticancer medications and/or complexes. In addition, knowing the phenyl esters' thermochemistry aids in the prediction and control of their membrane-crossing capabilities, their dispersion and disintegration in aqueous conditions, and how they interact with plasma proteins.

Enthalpy of solution

Enthalpy of solution, or heat of solution, is the amount of heat or enthalpy evolved or absorbed when a compound dissolves in a solvent at standard temperature and under a pressure of 0.1 MPa. In this work, solution enthalpy was determined for the phenyl ester compounds in benzene solvent using the adiabatic solution calorimetry technique at 298.15 K, and the values of enthalpy of solution for some compounds were predicted from the following Equations (2) and (3).
From Equation (2), it was obtained that the enthalpy of solvation;

$$\Delta_{solv}H^{Ai/S} = \Delta_{solv}H^{ArH/S} + \Sigma\,\Delta_{solv}H^{\mathrm{Xi}\rightarrow\mathrm{H}/S} \quad (2)$$

Where, $\Delta_{solv}H^{\mathrm{Xi}\rightarrow\mathrm{H}/S}$ is the solvation enthalpy of the substituent group in solvent S, and $\Delta_{solv}H^{ArH/S}$ is the solvation enthalpy of the basic compound without any attached groups in the same solvent S. All enthalpy values are at the same temperature.
Then, from Equation (3), the enthalpy of solution at standard temperature:

$$\Delta_{soln}H_m^{Ai/S}(298.15\ K) = \Delta_{cr,liq}^{g}H_m^{Ai}(298.15\ K) + \Delta_{solv}H_m^{Ai/S}(298.15\ K) \quad (3)$$

Where $\Delta_{soln}H_m^{Ai/S}(298.15\ K)$ is the enthalpy of solution of compound *Ai* in solvent *S* at temperature 298.15 K, $\Delta_{cr,liq}^{g}H_m^{Ai}(298.15\ K)$ is the enthalpy of evaporation of compound *Ai* at mean temperature *m* and $\Delta_{solv}H_m^{Ai/S}(298.15\ K)$ is the enthalpy of solvation for sample *Ai* to solvent *S* mean temperature 298.15 K.

The heat of solubility, or enthalpy of solution, for the phenyl ester compounds in the benzene solvent was estimated at a temperature of 298.15 K. Table 2 represents the solution enthalpy values for the attached groups to the phenyl esters, and the values ranged from 0.05 to 41.8 kJ/mol with respect to the attached groups to the phenyl ester parent compound. The enthalpies for the methyl p-fluorobenzoate and methyl benzoate in benzene solvent are close to each other by the value of 0.46 kJ/mol and 0.37 kJ/mol respectively, that's due to the fluorine and hydrogen atoms substituted in the para position due to significantly atomic size effect as well as solvent affect (benzene solvent was used in this work therefore the fluorine substitution has not impact). In addition, the solution enthalpies for the compounds methyl p-chlorobenzoate, methyl p-bromobenzoate, and methyl p-aminobenzoate are also close to each other in the enthalpy values; however, they differ in atomic properties, but they are similar in molecular size. The estimated value for the ethyl benzoate compound agrees well with the value mentioned in the reference [16]. The highest value of solution enthalpy for propyl p-hydroxybenzoate is due to the attached hydroxy group and the substitution of a propyl group in the other direction of the molecule, which makes it difficult to dissolve in benzene solvent. Then, the enthalpy of solution value for n-butyl benzoate is lower due to easy dissolution in benzene solvent. Finally, the substituted groups in the para position in the phenyl esters are dominated by the size of the substituted groups; however, polarity plays a role in another way.

Table 2. Enthalpy of solution of the Phenyl esters in S solvent (kJ/mol) at 298.15 K.

Compound	$\Delta_{soln}H_m^{Ai/S}$	Ref.
Methyl 4-fluorobenzoate	0.46 ± 0.24	This work
Methyl 4-chlorobenzoate	24.36 ± 0.33	This work
Methyl 4-bromobenzoate	25.37 ± 0.19	[17]
Methyl 4-aminobenzoate	25.52 ± 0.29	This work
Phenyl acetate	3.23 ± 0.18	This work
Methyl benzoate	0.37 ± 0.05	[18]
Methyl phenyl acetate	0.12	[19]
Ethyl benzoate	0.05, 0.55 [a]	[16]
Ethyl 4-hydroxybenzoate	28.85 [a]	This work
n-Propyl benzoate	12.32 [a]	This work
Propyl 4-hydroxybenzoate	41.8 [a]	This work
n-Butyl benzoate	1.05 [a]	This work

[a] Values estimated from the predicted values of solvation enthalpies in this work and the average value of the evaporation enthalpies from Table 4 and the enthalpy of solvation Equations (2 and 3).

Enthalpy of solvation

Additive scheme approach

The additive scheme approach is a simple way to estimate the solvation enthalpy of the organic aromatic compounds in the various solvents mentioned in Solomonov's article [18]. Correspondingly, the approach was applied to calculate the enthalpy of solvation for various organic aromatic compounds [6, 7, 13, 20] at standard temperature 298.15 K. The additive scheme approach is based on summing the substituted group with the parent compounds according to the following Equation;

$$\Delta_{solv}H^{\mathrm{X\rightarrow H}/S} = \Delta_{solv}H^{ArX/S} - \Delta_{solv}H^{ArH/S} \quad (4)$$

Where $\Delta_{solv}H^{\mathrm{X\rightarrow H}/S}$ is the solvation enthalpy of the substituent group in solvent *S*, $\Delta_{solv}H^{ArH/S}$ is the solvation enthalpy of the parent compound without any attached groups in the same solvent *S*, and $\Delta_{solv}H^{ArX/S}$ is the enthalpy of solvation for the parent compound with the attached X substituted group in solvent S. With respect to this approach, the solvation enthalpy for functional groups was estimated according to Solomonov and his co-authors' approach [18] (Table 3). Besides, the enthalpy of solvation for the group's ethyl, propyl, butyl, and carboxylate groups was estimated in this work.

Table 3. Solvation enthalpy (kJ/mol) in benzene solvent for the contributing groups.

Group	$-\Delta_{solv}H^{Ai/Bz}$
CH_3-	3.5[a]
F-	-0.4 [a]
Cl-	6.1 [a]
Br-	8.6 [a]
-NH_2	15.8 [a]
-$COOCH_3$	20.4 [a]
-OH	14.4 [a]
CH_3CH_2-	7.3 [b c]
$CH_3CH_2CH_2$-	12.3 [b c]
$CH_3CH_2CH_2CH_2$-	16.33 [b c]

-COO-	16.9 [c]

[a] Values were taken from reference [18] (additive scheme approach). [b] the approximated value was obtained according to Equation (3). [c] the values are predicted in the present study.

Solution calorimetry method

In addition, solution calorimetry was applied for estimating the enthalpy of solvation of phenyl esters in benzene solvent at 298.15 K, according to the following Equation;

$$\Delta_{solv}H^{Ai/S} = \Delta_{soln}H_m^{Ai/S} - \Delta_{cr,l}^{g}H_m^0 \quad (5)$$

Utilizing the solution calorimetry technique at 298.15 K, the enthalpy of solution for the chemicals listed in Table 2 was found. After gathering the enthalpy of sublimation/vaporization from average values of the same chemicals at standard temperature 298.15 K from literature data, the enthalpy of solvation value was observed for phenyl esters in benzene solvent with respect to Equation (5). To emphasize the values, the enthalpy of solvation was calculated using another method named the Abraham model.

Abraham model

Abraham model is a computational model with solute and solvent descriptors. The solute descriptors involve constructing a series of mathematical expressions for the measured solute properties of the given solute in a series of solvents and/or for a series of processes for which the lowercase Equation coefficients are known. The solvent descriptors were evaluated in the Equation with respect to reference [21]. Accordingly, chemists applied the Abraham model [22]. The solute descriptors are in capital letters and the solvent descriptors in small letters. The Abraham model is satisfied according to the following Equations:

$$\Delta_{solv}H^{Ai/S} = c + e\,\boldsymbol{E} + s\boldsymbol{S} + a\boldsymbol{A} + b\boldsymbol{B} + l\boldsymbol{L} \quad (6)$$

$$\Delta_{solv}H^{Ai/S} = c + e\,\boldsymbol{E} + s\boldsymbol{S} + a\boldsymbol{A} + b\boldsymbol{B} + v\boldsymbol{V} \quad (7)$$

The solute descriptors: E is represented as the excess molar refraction in cm^3/mol.10, **S** indicates the solute dipolarity/polarizability, **A** is the overall solute hydrogen bond acidity, **B** refers to the overall solute hydrogen bond basicity, V is McGowan's property of molecular volume in cm3/mol.100, and L is calculated as the logarithm of the gas-to-solvent S at 298 K.

The complementary solvent properties in Equations (5) and (6) are given by the lowercase alphabetical characters (c, e, s, a, b, v, and l). Numerical values of the solvent properties are determined by regressing measured data for a series of solutes with known descriptor values. Once estimated, the lowercase alphabetical characters allow one to predict the specified property of additional solutes in the given solvent, provided of course that the solute descriptors are known. The Abraham solvation parameter model has been described in greater detail in several published papers, book chapters, and review articles [23]. By the way, this model requires knowing many chemical properties of the solute and solvent molecules. It is better to know some lower measurements and chemical properties, such as the molar refraction method.

Moreover, the solvation enthalpy for the phenyl esters was calculated in benzene solvent according to Equations (8) and (9). The solvent descriptors were evaluated using the Equation with respect to the reference [21]. The solute descriptors were collected from the chemical properties ChemSpider website [24], [25], [26], [27]. The observed values of solvation enthalpy were listed in Table 4.

$$\Delta_{solv}H^{Ai/Bz} = -4.637 + 4.446\,\boldsymbol{E} - 12.599\boldsymbol{S} - 9.775\boldsymbol{A} - 4.023\boldsymbol{B} - 8.488\boldsymbol{L} \quad (8)$$

$$\Delta_{solv}H^{Ai/Bz} = -4.637 + 4.446\,\boldsymbol{E} - 12.599\boldsymbol{S} - 9.775\boldsymbol{A} - 4.023\boldsymbol{B} - 8.488\boldsymbol{V} \quad (9)$$

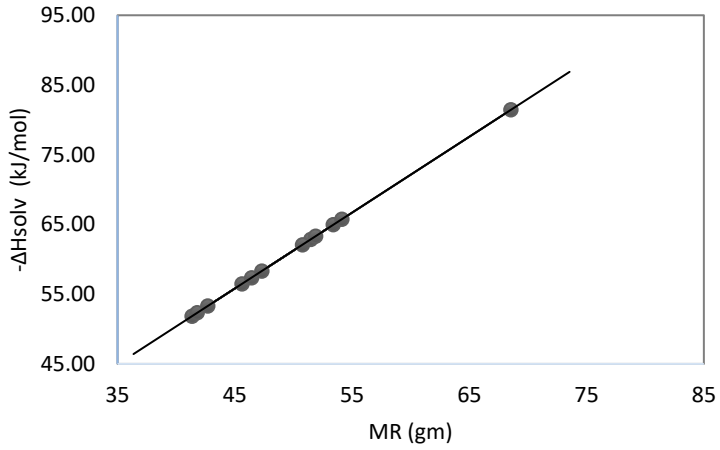
Where $\Delta_{solv}H^{Ai/Bz}$ is the enthalpy of solvation of *Ai* compound in benzene solvent *Bz* [22]. The above method mostly depends on atomic properties, and it is a theoretical model. Therefore, it's more favorable to present another experimental approach to obtain values that agree well with each other and are acceptable to scientists, such as the molar refraction method.

Molar refraction method

In another way, according to the molar refraction method, the enthalpy of solvation was calculated from the following Equation according to reference [28];

$$-\Delta_{solv}H^{Ai/Bz} = 6.86 + 1.08\ MR^{Ai} \qquad (10)$$

Where MR^{Ai} is the molar refraction of the solutes Ai; in this work, it was calculated by multiplying the molar refractivity and density (from the ChemSpider website [26], [27], [29]) of the compounds studied in this work. The values indicated in the below figure and table (4). While, the standard deviation is due to the other methods used in this work.



(N=20, R=1, SD=2.29)

Figure 2. The molar refraction- enthalpy of solvation relation with respect to Equation (8).

The solvation enthalpy values were obtained from the methods mentioned above: additive scheme approach, solution calorimetry, Abraham model, and molar refraction at a temperature of 298.15 K in benzene solvent; all values were presented in Table 4.

The enthalpy of solvation values of the phenyl esters in this study vary from about 55 kJ/mol to 80 kJ/mol according to their chemical structure compositions and the methods applied to determine them. The values of solvation enthalpy for methyl 4-fluorobenzoate, phenyl acetate, methyl phenyl acetate, and methyl 4-chlorobenzoate are about 55 kJ/mol, and there is no significant difference among the methods, as well as the values have low standard deviations. While the solvation enthalpy for n-butyl benzoate and methyl 4-bromobenzoate has large values of the standard deviation due to the Abraham model method, n-butyl benzoate has a high molecular mass, and the molar refraction method gives a high value of solvation enthalpy compared to the other methods. Nevertheless, the compounds methyl 4-aminobenzoate, n-propyl benzoate, and propyl 4-hydroxybenzoate respectively have high values of enthalpy of solvation due to the attached groups: carboxyl, hydroxyl, and amino groups; they have high polarity on the benzene ring side for the esters. Additionally, the compounds attached to n-propyl and n-butyl

groups were made into molecules in which these molecules are more than others. Despite this, the largest deviation of the solvation enthalpy values due to the Abraham model and molar refraction methods for methyl 4-bromobenzoate and n-butyl benzoate was 81.44 kJ/mol and 81.58 kJ/mol, respectively. These methods depend on molecular properties and the molar refractivity of the molecules.

Table 4. Solvation enthalpies of the Phenyl esters in S solvent (kJ/mol) at 298.15 K.

Compound	$-\Delta_{solv}H_m^{Ai/S}$ [a]	$-\Delta_{solv}H_m^{Ai/S}$ [b]	$-\Delta_{solv}H_m^{Ai/S}$ [c]	$-\Delta_{solv}H_m^{Ai/S}$ [e]	$-\Delta_{solv}H_m^{Ai/S}$ [f]
Methyl 4-fluorobenzoate	54.8	55.51	55.26	56.47	55.51±0.61
Methyl 4-chlorobenzoate	61.3	60.17	63.86	62.87	62.05±1.42
Methyl 4-bromobenzoate	63.9	63.93	68.01	81.44	69.32±7.19
Methyl 4-aminobenzoate	71	75.09	57.77	62.09	66.49±6.89
Phenyl acetate	52.4	50.99	50.70	51.86	51.49±0.68
Methyl benzoate	58.7	53.65	55.47	52.34	55.04±2.39
Methyl phenyl acetate	55.9	57.28	57.64	57.36	57.045±0.67
Ethyl benzoate	59.0 [d]	57.54	64.30	53.32	58.54±3.93
Ethyl 4-hydroxybenzoate	73.4 [d]	-	64.34	64.96	67.57±4.13
n-Propyl benzoate	64.0 [d]	-	72.73	58.32	65.02±5.93
Propyl 4-hydroxybenzoate	78.4 [d]	-	71.4	65.74	71.85±5.18
n-Butyl benzoate	68.03 [d]	-	81.58	63.33	70.98±7.74

[a] The values were calculated by the additive scheme method, [b] the values were measured from Equation (5) (evaporation enthalpy collected from the average value of evaporation enthalpy at 298.15 K from table (5) and the value experimentally estimated table (1)). [c] the values were calculated by the Abraham model. [d] values were estimated from the predicted values of solvation enthalpies in this work and the average value of the evaporation enthalpies from Table (5). [e] the values are predicted by the molar refraction method. [f] the average values are collected for the methods with standard deviations.

Enthalpy of vaporization/sublimation

In this work, the sublimation/vaporization enthalpy was determined for six compounds using the solution calorimetry method in benzene and/or acetonitrile solvents at 298.15 K.
The sublimation enthalpy for the crystalline compounds is calculated from fusion enthalpy and vaporization enthalpy as follows;

$$\Delta_{cr}^{g}H_m^0 = \Delta_{cr}^{liq}H^{Ai} + \Delta_{liq}^{g}H_m^0 \quad (11)$$

According to the above Equation and using the solution calorimetry-additive scheme approach, the enthalpy of sublimation/vaporization of the phenyl esters at temperature 298.15 K was determined. The enthalpy values in this work were compared to those of the literature data. The enthalpy values from literature data at temperatures higher than 298 K were then adjusted to the standard temperature 298.15 K using the Kirchhoff law:

$$\Delta_{cr,liq}^{g}H_2 = \Delta_{cr,liq}^{g}H_1 + \Delta_{cr,liq}^{g}C_p * (T_2 - T_1) \quad (12)$$

The heat capacity from the above Equation was calculated using the following Equations with respect to the state of the compounds [30];
For the liquid compounds applied:

$$\Delta_{liq}^{g} C_p = 10.58 + 0.26\, C_p(liq) \quad (13)$$

For the crystalline compounds applied:

$$\Delta_{cr}^{g} C_p = 0.75 + 0.15\, C_p(cr) \quad (14)$$

Accordingly, the values of sublimation/vaporization enthalpies measured in this work agree well with the literature data. Accurately, the average values (bolded values in Table 5) are calculated from literature data and observed values in this work at a temperature of 298.15 K. In addition, the standard deviation was set for all the average values of the enthalpy of evaporation of the studied compounds. Moreover, the evaporation enthalpy values of the compounds Methyl 4-fluorobenzoate, Methyl 4-chlorobenzoate, Methyl 4-bromobenzoate, Phenyl acetate, and Methyl benzoate were in the best agreement with the literature values. Furthermore, the enthalpy values have the lowest standard deviation, which is no more than ±1.6 kJ/mol. While the sublimation enthalpy values for Propyl 4-hydroxybenzoate, Methyl 4-aminobenzoate, and Ethyl benzoate compounds have a high standard deviation due to the difficulty of studying these compounds, and they are sparingly soluble in benzene solvent. However, sublimation enthalpy for methyl 4-aminobenzoate compound was measured in this work value was 96.52 kJ/mol by solution calorimetry-additivity scheme method at 298.15 K. Nevertheless, the values of sublimation enthalpy for Methyl 4-aminobenzoate were 103.4 ± 0.2 kJ/mol [31], 101.1 kJ/mol [32] and 104.2 ± 0.3 kJ.mol^{-1} [31] by static, fusion enthalpy-solvation enthalpy and Mass effusion-Knudsen effusion respectively. However, in this work, the enthalpy value was in poor agreement with literature values. Therefore, the additive scheme is weakly applicable for highly polar compounds[18]. Similarly, the sublimation enthalpy for the hydroxy phenyl ester compounds Ethyl 4-hydroxybenzoate and Propyl 4-hydroxybenzoate, which are high-polarity compounds in the crystalline state, therefore has approximately the same reasons as the methyl 4-aminobenzoate compound as mentioned above. While the enthalpy of vaporization for the compounds Ethyl benzoate, Propyl benzoate and n-Butyl benzoate were determined H. Katayama (at 1988) [33] through the Bourdon gauge method and vapor pressure methods at reduced pressure their average value enthalpy of vaporization are 58.45, 51.68 and 69.06 in kJ/mol respectively, where they are in liquid state and low polarity and they are in weak intermolecular interaction. Granted, the sublimation enthalpy results agree well with each other, and they have lower standard deviation values.

Table 5. Evaporation enthalpy of the studied compounds by various methods.

Compound	M[a]	T/K range (Tm) [b]	$\Delta_{cr,liq}^{g} H_m^o$ kJ.mol^{-1}	$\Delta_{cr,liq}^{g} H_m^{Tm}$ kJ.mol^{-1}	Ref.
Methyl 4-fluorobenzoate (*liq*)	SC	298.15	56.2		[34]
	S	268.6-344.8	56.0	56.0 ± 0.1	[35]
	S	269-344(307)		55.4 ± 0.1	[35]
	SC	298.15	56.4		[36]
	SC	298.15	55.26 ± 0.24 [e]		This work
			55.97 ± 0.50 [d]		Average
Methyl 4-chlorobenzoate (*cr*)	S	277-312(295)		83.5 ± 0.1	[35]
	S	277-312	83.4 ± 0.1		[35]
	S	285-334(310)		61.6 ± 0.1 [c]	[35]
	S	285-334		62.4 ± 0.1 [c]	[35]

	SC	298.15		62.5 [c]	[36]
	SC	298.15	85.66 ± 0.33 [e]		This work
			84.53 ± 1.60 [d]		Average
Methyl 4-bromobenzoate (*cr*)	S	293-349 (321)		88.7 ± 0.1	[35]
	S	293-349	89.3 ± 0.2		[35]
	S	355-378(367)		60.6 ± 0.2	[35]
	SC	298.15		65.1 [c]	[36]
	S	355-378		66.1 [c]	[35]
	SC	298.15	89.27		This work
			89.29 ± 0.02 [d]		Average
Methyl 4-aminobenzoate (*cr*)	S	333-380	103.4 ± 0.2		[31]
	FS	298.15	101.1		[32]
	MK	319-341	104.2 ± 0.3		[31]
	S	333-380(356)		101.7 ± 0.2	[31]
	S	361-428(294)		74.5 ± 0.1 [c]	[31]
	S	361-428	84.0 ± 0.1 [c]		[31]
	SC	298.15	96.52 ± 0.19 [e]		This work
			100.61 ± 3.86 [d]		Average
Phenyl acetate (*liq*)	CGC	433-473	53.58		[37]
	A	326		51.7	[38]
	CGC	313- 363	53.3		[37]
	CGC	313. - 353	53.1		[37]
	C	298.15	55.2 ± 0.8		[39]
	V	298.15	54 ± 2		[40]
	N/A	298.15	54.8		[40]
	SC	298.15	55.58 ± 0.18 [e]		This work
			54.22 ± 0.98 [d]		Average
Methyl benzoate (*liq*)	CGC	333-433	57.4		[41]
	CGC	313-353	53.4		[37]
	CGC	313-353	53.8		[37]
	CGC	433-473	54.7		[37]
	A	283-323	53.9		[42]
	A	373-533(388)	53.82	49.7	[42]
	C	298	55.6 ± 0.1		[43]
	EB	358-517(360)	53.94	51.1 ± 0.2	[44]
	EB	358-517(400)		48.5 ± 0.2	[44]
	EB	358-517(440)		45.8 ± 0.2	[44]
	EB	358-517(480)	51.34	43.0 ± 0.4	[44]
	C	303		57.2 ± 0.1	
	SC	298.15	52.72 ± 0.05 [e]		This work
			53.69 ± 1.2 [d]		Average
Ethyl benzoate (*liq*)	GS	283-332	61.1 ± 0.3		[45]
	EB	369-531	56.85	52.5 ± 0.2	[44]
	EB	369-531		49.6 ± 0.2	[44]
	EB	369-531		46.7 ± 0.3	[44]
	EB	369-531		43.6 ± 0.5	[44]
	BG	344-440	60.13	57.0	[33]
	BG	344-440		50.5	[33]
	A	(288-333)		55.9	[38]
	A	358-487		50.4	[38]
	A	317-486	53.7 [g]	51.9	[46]
			58.45 ± 3.0		Average
Ethyl 4-hydroxybenzoate(*cr*)	GS	313-326	100.9 ± 0.7		[47]
	CGC	298	84.0 ± 0.5 [g]		[48]

	TGA		104.8 [f]	75.0	[49]
	TGA		102.4 [f]	72.6	[50]
			102.25 ± 1.8		Average
Propyl benzoate (*liq*)	BG	359-458	55.50	60.2	[33]
	BG	359-458	44.46 [g]	52.7	[33]
	A	327-504	51.25	53.8	[42]
			51.68 ± 2.3		Average
Propyl 4-hydroxybenzoate (*cr*)	GS	319-333	123.7 ± 0.6		[47]
	CGC		116.7 [f]	89.5 ± 0.6	[48]
	TGA		113.8 [f g]	79.1	[49]
	TGA		111.2 [f g]	76.5	[50]
			120.2 ± 4.9		Average
n-Butyl benzoate (*liq*)	BG	374-474(394)	70.58	63.2	[33]
	BG	374-474(452)	67.55	55.7	[33]
	A	343-405(358)	63.71 [g]	59.1	[38]
			69.06 ± 2.1		Average

[a] Methods; S=static method, SC= Solution Calorimetry, EB= ebulliometric method, A=calculated from the vapor pressure data reported by the method of least squares, C=calorimetry, CGC=correlation gas chromatography, MK=Mass effusion-Knudsen effusion, TGA= Thermal gravimetric analysis, GS=gas saturation, n, transpiration method, BG= Bourdon gauge method and FS= fusion enthalpy and solvation enthalpy. [b] T_m is mean temperature in the brackets (evaporation enthalpy calculated at T_m). [c] the values were measured for the liquid state. [d] the standard uncertainties were calculated from the standard deviation of evaporation enthalpy values at 298.15 K. [e] the evaporation enthalpy values in this work were measured by equations (1) and (3), the standard uncertainty calculated from solution enthalpy values. [f] the values are collected from summing enthalpy of fusion and enthalpy of vaporization. [g] the values were excluded from calculations of the average values.

The evaporation enthalpy values of the methyl para-substituted benzoates, methyl benzoate, ethyl benzoate, propyl benzoate, butyl benzoate, and phenyl acetate were obtained at 298.15 K in this work and from literature data. Consequently, the enthalpy of sublimation/vaporization values indicate the effect of the para position and isomer effect of the phenyl acetate and methyl benzoate (sublimation/vaporization, solvation, and solution enthalpies) of the studied compounds by substitution of the hydrogen atom at the para position with fluoro, chloro, bromo, amino, and hydroxyl groups (Figure 2). Moreover, the vaporization enthalpy values of the compounds methyl benzoate and phenyl acetate were investigated that the isomer phase transition enthalpy impact. Of course, the amino- and hydroxyl-substituted groups represented the most significant effect on the enthalpy values of sublimation, solvation, and solution enthalpies because they have high polarity and can make strong intermolecular interactions; therefore, methyl 4-aminobenzoate, Ethyl 4-hydroxybenzoate, and Propyl 4-hydroxybenzoate compounds had the highest values of solution, solvation, and sublimation enthalpies.

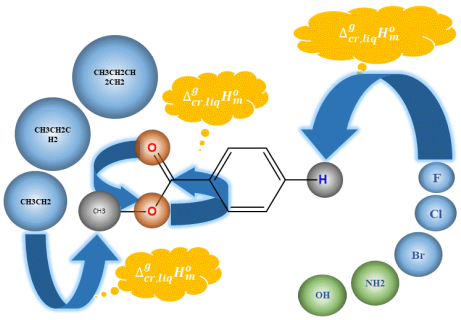


Figure 3. The chemical structure of phenyl ester derivatives.

Further, knowing the enthalpies of solvation and vaporization for the compound's phenyl acetate and methyl benzoate, the isomer effect is expected when exchanging the carboxyl group in the present phenyl group; it is not significant enough for the enthalpies of solvation and vaporization, but it may significantly affect applications in drug manufacturing.

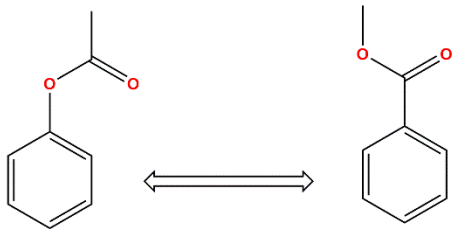


Figure 4. The chemical structure of methyl benzoate and phenyl acetate and their solvation enthalpy in blue color and enthalpy of vaporization in red color.

Hence, from the solution, solvation, and evaporation enthalpy values of the para-substituted methyl benzoate and phenyl acetate, the stability of the compounds was explained. Furthermore, the halogen and amino, as well as the hydroxyl-substituted groups in the presence of a carboxyl group, made a significant change in the enthalpy of solution, solvation, and evaporation values of the studied compounds in this work. Consequently, the application of these compounds in complexes for manufacturing anticancer drugs has quite a bit impacted their consumption by patients.

CONCLUSIONS

Enthalpies of solution, solvation, and evaporation were distinguished for the phenyl ester derivative compounds at 298.15 K. Accordingly, new values of solvation enthalpy were predicted for the substituted groups: ethyl, propyl, and butyl, through various methods. The enthalpies of para-substituted polar groups to the phenyl esters indicated the most stable compounds; then halogenated methyl benzoate compounds have lower energy compounds for solution, solvation,

and evaporation phenomena. Besides, any addition of hydroxide or amino groups to phenyl esters can make the compound more stable and harder to dissolve, especially in benzene solvent. Therefore, the phase change enthalpy values represent the energy and the stability of the studied compounds. Accordingly, the researchers can make decisions on choosing which molecules are better for producing material complexes and/or manufacturing drugs for anticancer cases.

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Declarations

The author has accepted publication of this article, and there is no known conflict of interest in this work.

Availability of data and materials

The data will be available upon request.

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