The Published Fusion Enthalpy and its Influence on Solubility Estimation for Alcohols

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Abstract: *This paper aims to compare two different methods of estimating enthalpy of fusion and identify the one which is closer to the already published value. The n-long chain alcohols such asn-octanol(C_8), dodecanol(C_{12}), tridecanol(C_{13}), tetradecanol(C_{14}), pentadecanol(C_{15}), hexadecanol(C_{16}), heptadecanol(C_{17}), octadecanol(C_{18}), nonadecanol(C_{19})and eicosanol(C_{20})were the systems used for testing the methods. The experimental or estimateddata was available in the literature, and comparisons enabled the determination of the relative deviations for the compounds studied. It was expected that the enthalpy of fusion could be well evaluated by using sublimation and vaporization enthalpy as well as with the use of liquid and solid enthalpies of formation for the compound. However, when the results were compared with the literature ones, it was found that there are problems with the data published (experimental or not) because of the high relative deviations presented. Then, the prediction of solid-liquid equilibrium (SLE)had errors due to the high inconsistencepresented by this thermophysical property specially for C_{14}, C_{15}, C_{16} and C_{18}. Thefirst method, which used the liquid and solid enthalpy of formationcan be used without restrictions and the second one had a better estimative of fusion enthalpy justfor some of the alcohols tested.*

Keywords: *fusion; enthalpy; published data; solubility; estimation; solid-liquid.*

1. INTRODUCTION

Alcohols with long chain have long been an interesting class ofcompounds for the chemist. A casual examination of the literature shows the important applications on solvents, additives, drugs and dyes [1,2].

Experimental or estimated results of thermodynamic properties of sublimation and vaporization enthalpy of several long chain alcohols have been reported by researchers [1–12]. Also, heat of formation of them in the liquid and solid phase are available. Inthis work these data are appliedin two differents equations to calculate enthalpy of fusion. Moreover, it could be possible to verify ifthe experimental data for fusion enthalpy available in NIST - National Institute of Standards and Technology (https://webbook.nist.gov/chemistry)can be considered reliable for using in projects purpose.

The very important thermodynamic property named as standard enthalpy offusion or latent heat offusion (ΔH_i^{fus})has been defined as the enthalpy change in the transition from the most stable form of solid to liquid state at the normal melting point. It is required for calculation of energy balances in many operations in which solid–liquid phase changes may carry on. Commercial differential scanning calorimeter is also calibrated in situ using the reported standard molar entropy for some compound.Accuracy tests were already performed with n-decane and others hydrocarbons. Furthermore, ΔH_i^{fus} can be used to figure out other physical or chemical properties. One important property determined using enthalpy of fusion is the solubility of compounds in various solvents [2]. The enthalpies of fusion can be measured by different techniques such as isothermal calorimetry and by correlation gas chromatography. However, these are an indirect methods whose output strongly depends on data for reference compounds used.Bondi [3] was the first researcher who estimated ΔH_i^{fus}.

Then, he used this one in the following equation:

$$\Delta H_i^{fus} = T^{fus}\Delta S_{tm}^{fus} \tag{1}$$

Bondi [3] proposed application of total entropy of fusion at $0K\Delta S_{tot(0)}^{fus}$ instead of ΔS_{tm}^{fus} in Eq. (1). The equality of $\Delta S_{tot(0)}^{fus}$ and ΔS_{tm}^{fus} is true just for those compounds that do not have solid–solid transitions. For the compounds, Eq. (1) is a good proposal to give an estimation for ΔH_i^{fus}. Nevertheless, for the compounds that have solid–solid transitions, $\Delta S_{tot(0)}^{fus}$ is much greater than ΔS_{tm}^{fus}. This approach has been recently applied to account the total phase change enthalpy of more than 1000 pure compounds [4]. In another attempt, Marrero and Gani [5], developed several Group Contribution (GC) methods. They proposed a first order, a second order and a third order group contribution methods to estimate the fusion enthalpy. Their third order GC method showed the best results over 741 compounds they studied. The model showed standard deviation, average absolute error, average relative deviation of 3.65, 2.17 kJ.mol^{-1} and 15.7%. The quantitative structure–property relationship (QSPR) method has been utilized to predict the ΔH^{fus}. The QSPR-based methods were often used to predict the ΔH^{fus} of particular chemical categories of compounds [6–10]. No additional comments will be done about these methods because they were proposed for especial purposes and cannot be applied for general chemicals.

An evaluation of published (experimental or predicted) fusion enthalpy data for long chain alcohols will be done. The main goal of this work is to decide which method is the best for estimation of ΔH_i^{fus} of pure alcohols (C_8-C_{20}) related to the biofuel field of research. The method chosen probably will be confirmed by using the appropriate ΔH_i^{fus} data in the solid-liquid equilibrium (SLE) calculations. This work also shows that this property has strong influence on the solubility predictions, and the criterion for choosing which value to be used, has an important role in the final result.

2. METHODOLOGY

The enthalpy of fusion (ΔH_i^{fus}), as an important property for prediction of melting point and solubility of organic compounds [11-13], is related to the entropy of fusion (ΔS_{tm}^{fus}) and fusion point temperature (Tfus) because the Gibbs energy of transition is zero at the phase transition temperature, as already illustrated in Equation (1).

Some reliable simple methods have been recently developed to predict fusion temperature for different classes of compounds [14–18]. Different approaches can be used for estimating ΔH_{tm}^{fus} and ΔS_{tm}^{fus} at the melting point of some classes of organic compounds [19–27]. For compounds containing a benzene ring that easily bend, the value of ΔS_{tm}^{fus} on the basis of Walden's rule is constant with a value of 56.5 J.K-1 mol-1 [28, 29].

The purpose of this work is to use known methodologies associated with the experimental data to check the results, experimental or estimated, of enthalpy of fusion already published in NIST for long chain alcohols. It is believed that this method will be helpful when this thermophysical property has to be used in solid-liquid equilibria calculations. The prediction of SLE can be really led to errors when this variable is not properly determined in reliable way, then some calculations using experimental fusion enthalpy for the same compound will show that researchers in general have not to rely on them. This first manuscript is related to long chain alcohols used in the biofuel field of research. In other manuscript, we are presenting other compounds including acids and esters with long carbon chain.

The first method is based on the knowing of liquid and solid enthalpies of formation for the i compound. Therefore, the enthalpy of fusion is stated as:

$$\Delta H_{fus} = \Delta H_f^L - \Delta H_f^s \tag{2}$$

Where "ΔHfus" is the enthalpy of fusion, "ΔH_f^L" and "ΔH_f^s" are the liquid and solid enthalpy of formation, all of them in (kJ/mol).

For the second method the property of function of state will be applied. Then, in case of enthalpy, the way for sublimation is the samewhen going to fusion and after that to vaporization, as given by Equation (3):

$$\Delta H_{fus} = \Delta H_{sub} - \Delta H_{vap} \tag{3}$$

Where"ΔH_{sub}" and "ΔH_{vap}" are the sublimation and vaporization enthalpies. All data were collected from the literature and the calculated results are published in Tables 2-8.

In Table 1, data collected for C13- C19are presented and it is observedthat the discrepancies in the experimental ΔH_{fus}obtained in the same temperature in different periods. Then, it is clear that one method has to be used to confirm or to select the most reliable enthalpy of fusion for this class of compounds.

Calculated data will be done using Equation (3) and compared to the published (experimental or not) data reported in the literature. In Tables 2-7, the relative deviation(DR%) is related to experimental enthalpy of fusion and can be given as follows:

$$RD(\%) = \frac{\Delta H_{fus}^{pub} - \Delta H_{fus}^{calc}}{\Delta H_{fus}^{pub}} \times 100 \tag{4}$$

Where "ΔH_{fus}^{pub}" and "ΔH_{fus}^{calc}"are the published (experimental or not) and calculated enthalpy of fusion experimental, respectively, both in (kJ/mol).

3. RESULTS AND DISCUSSION

The predicted values of ΔH_{fus}^{calc}using the first method (Eq.2) are shown in Table 1, and for thesecond method, or Equation (3), in comparison with the published (experimental or predicted) data are depicted in Tables 2-8. Thermodynamic data available in the literature (NIST) were compared with estimative using the universal method and the results evaluated. The values of the predicted ΔHf us as well as the experimental data for sublimation and vaporization enthalpy are also presented in the ones. The discrepancies or deviations are presented in Table 1. Figure1is added here to discuss the accuracy of the published data available in the literature.

Table 1 and Figure 1 illustrate the discrepancy and deviation for fusion enthalpy already determined in laboratory and published as well. For this class of long chain alcohols, it is observed a high discrepancy in the available data published in literature. Table 2-7 will show that it is also occur for vaporization enthalpy. Therefore, in some cases, Equation (3) will present a weekly, or not reliable, estimative for the enthalpy of fusion. In spite of being not reliable for calculating of fusion enthalpy for some alcohols, we can recommend the Eq. (3) in case of the reliability of the experimental vaporization and sublimation data.
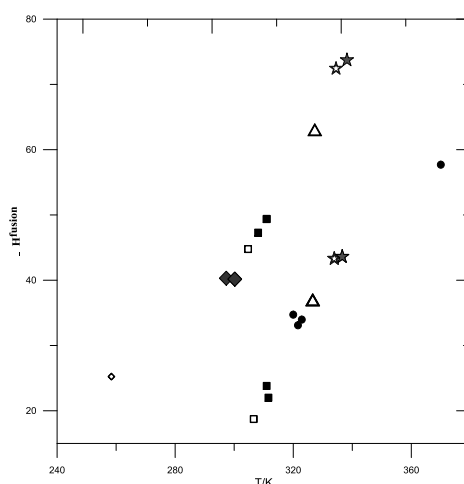

Fig1. *Published fusion enthalpy for C_8, C_{12}, C_{13}, C_{14}, C_{16}, C_{17}, C_{19} and C_{20}.*

Table1. *Published and calculated fusion enthalpy for C_{13}-C_{19} in (kJ/mol) ***(Compounds that there is no ΔH_{exp}^{sub} available to apply Eq. (3).)(* calculated by Equation (2) using enthalpy of formation extrapolated from C_4 to C_{10} published by NIST)*

Compound**	ΔH_{pub}^{fus}	T /K	Reference
1-tridecanol	44.78	304.7	van Miltenburget al., 2003[30]
	18.74	306.6	Mosselman, Mourik, et al., 1974[31]
tetradecanol	50.2*	298.15	This work – Eq. 2

	23.64	316.	Mosselman and Mouric, 1974	
1-Pentadecanol	54.73	316.6	Mosselman and Mouric, 1974	
	29.6	316.4	Ventolá et al., 2004[32]	
	53.62	316.9	van Miltenburg et al., 2003[30]	
	58.5*	298.15	This work– Eq. 2	
Hexadecanol	62.0*	298.15	This work– Eq. 2	
1- Heptadecanol	37.0	326.6	Ventolá et al., 2004[32]	
	63.06	327.3	van Miltenburget al., 2003[30]	
	37.0	326.6	Ventolà et al., 2004[32]	
Octadecanol	62.8*	298.15	This work– Eq. 2	
1-nonadecanol	43.3	333.9	Ventolá et al., 2004[32]	
	72.42	334.5	van Miltenburget al., 2001[33]	

Table2. *Published and calculated enthalpiesfor 1-octanol. (kJ/mol)*

ΔH_{pub}^{fus}	T /K	Reference	ΔH_{cal}^{fus} This work	T /K	RD(%)
25.24	258.4	van Miltenburget al.,	37.8	258.4	49.8
ΔH_{exp}^{vap}	T /K	Reference	ΔH_{exp}^{sub}	T /K	Reference
69.6	282. - 321.	Kulikov et al., 2001[35]	100.4	468.	Davies and Kybett, 1965[37]
68.7	273. - 363.	N'Guimbi et al., 1992[36]			
64. ± 1.	267.	Davies and Kybett, 1965[37]			
62.6	258.4	This work			

It is believed that there is a problem with the sublimation enthalpy due to vaporization data seems to be reliable in the period of 1965-2001. Then fusion enthalpy could be regarded as reliable in terms that additional information of sublimation enthalpy must be provided to check by using the Equation 3.

Table3. *Published and calculated enthalpies for Dodecanol.*

ΔH_{pub}^{fus}	T /K	Reference	ΔH_{cal}^{fus} This work	T /K	RD(%)
40.31	297.3	van Miltenburget al., 2003 [30]	37.6	289.5	6.7
40.17	300.2	Acree, 1993 [38]			6.4
ΔH_{exp}^{vap}	T /K	Reference	ΔH_{exp}^{sub}	T /K	Reference
85.8	303. - 348.	Kulikov et al., 2001[35]	130.1 ± 1.2	285. - 294.	Davies and Kybett, 1965[37]
83.3	303. - 363.	Stephenson and Malanowski, 1987[39]			
95. ± 2.	297.	Davies and Kybett, 1965[37]			
97.3	289.5	This work			

Table4. *Published and calculated enthalpies for 1-tetradecanol.*

ΔH_{pub}^{fus}	T /K	Reference	ΔH_{cal}^{fus} This work	T /K	RD*(%)	RD**(%)
49.400	311.	N/A	37.5*	311.	24.1	1.8
47.29	308.1	Zeng et al., 2009[40]	50.3**	311.	20.7	6.4
23.81	311.	Mosselman and Mouric, 1974[31]	* Calculated using data from Wilhoit and Zwolinski, 1973 ** Calculated using data from Kulikov et al., 2001		59.0	111.

22.01	311.6	Mosselman and Mouric, 1974[31]			70.4	129.
49.37	311.	Mosselman and Mouric, 1974[31]			24.1	1.9
ΔH_{exp}^{vap}	T /K*	**Reference**	ΔH_{exp}^{sub}	T /K*	**Reference**	
106.4	313. - 358.	Wilhoit and Zwolinski, 1973[41]	143.9	293. - 307.	Davies and Kybett, 1965	
104.2	313. - 326.	Davies and Kybett, 1965[37]				
93.6	312. - 346.	Kulikovet al., 2001[35]				

Table5. *Published and calculated enthalpies for Hexadecanol*

ΔH_{pub}^{fus}	T /K	**Reference**	ΔH_{cal}^{fus}	T /K	**RD(%)**
57.7	80. - 370.	Xinget al., 2008[42]	57.7	453.2	7.1
33.1	321.6	Ventolá et al., 2004[32]	53.6	321.5	61.9
33.97	322.9	Kuchhalet al., 1979[43]			57.8
34.727	320.	Eykman, 1889[44]			54.3
ΔH_{exp}^{vap}	T /K	**Reference**	ΔH_{exp}^{sub}	T /K	**Reference**
107.7 ± 1.2	453.2	Nichols et al., 2006[45]	169.5 ± 2.5	453.2	Gundry, Harrop, et al., 1969
108.8	453.2	Kulikov et al., 2001[35]	169.6	453.2	Gundry, Harrop, et al., 1969
112.5	453.2	Ovaet al., 2000[46]	167. ± 2.	453.2	Davies and Kybett, 1965
100.4	328. - 362.	Kulikov et al., 2001[35]	169.5 ± 2.1	453.2	Davies and Kybett, 1965
109.4	323. - 335.	Stephenson and Malanowski, 1987[35]	167.4 ± 2.1	308. - 320.	Davies and Kybett, 1965
113.8	321.5	Interpolated into data for this work			

It seems that data published   between 1889 and 2004 are really suspicious and not reliable to be used in calculations of solid-liquid equilibria (SLE). This comment could be applied for 1-Pentadecanol entirely and will be checked at the end of this work.

Table6. *Published and calculated enthalpies for Octadecanol($C_{18}H_{38}O$). (kJ/mol)*

ΔH_{pub}^{fus}	T /K	**Reference**	[1]ΔH_{cal}^{fus} This work	T /K	**RD(%)**
40.1	330.1	Ventoláet al., 2004[32]	69.2	323.5	72.6
40.1	330.3	Ventolà et al., 2004[32]	69.2	318-330	72.6
66.67	331.2	van Miltenburg et al., 2001[30]			3.8
70.08	334.2	Chickoset al., 1991			1.3
ΔH_{exp}^{vap}	T /K	**Reference**	ΔH_{exp}^{sub}	T /K	**Reference**
86.4	435. - 504.	Stephenson and Malanowski, 1987[39]	187.4 ± 1.3	318. - 329.	Davies and Kybett, 1965[37]
76.3	500. - 573.	Stephenson and Malanowski, 1987[39]			
113.5	334. - 356.	Stephenson and Malanowski, 1987[39]			
118.2*	323.5	Interpolated for this work.			

Table7. *Published and calculated enthalpiesfor eicosanol. (kJ/mol)*

ΔH_{pub}^{fus}	T /K	**Reference**	[1]ΔH_{cal}^{fus} This work	T /K	**DR(%)**
43.6	336.6	Ventolà et al., 2004[32]	97.4	338.2	129.
43.6	336.6	Ventolàet al., 2004[32]	102.4	338.2	129.

ΔH_{exp}^{vap}	T /K*	Reference	ΔH_{exp}^{sub}	T /K*	Reference
73.72	338.2	van Miltenburg et al., 2001[30]	99.9*	338.2	35.5
		* Average value between data fromVentolá et al., 2004.			
83.5	488. - 653.	Stephenson and Malanowski, 1987[39]	218. ± 3.8	327. - 341.	Davies and Kybett, 1965
83.4	493. - 648.	Stephenson and Malanowski, 1987[39]	223. ± 3.8	T_{eb}	Davies and Kybett, 1965
118.9	339. - 358.	Stephenson and Malanowski, 1987[39]			
120.6	336.	Interpolated into data for this work			
120.4	338.	Interpolated into data for this work			

Teb – Normal temperatureof vaporization (1 atm)

In general, relative deviation stayed between 1.0 and 130%. This result is lower than whenenthalpy of is estimated using contribution methods. Not considerable amount of experimental data is available to test the methodology, despite of it more experimental efforts must be done for this class of compounds to check the vaporization and sublimation enthalpies published.

The study of experimental enthalpy of fusion for long chain alcohols (C8-C20) has confirmed that the suitable method employed had an important role showing that there are problems with the fusion enthalpy data published in literature. It was also indicated that the presence or absence of some experimental data such as sublimation enthalpy should be considered. Further investigations for the same compounds and taking into account compounds containing different types of groups have to be done.

The most results shown that the contribution of the vaporization enthalpy in prediction of the enthalpy of fusion is large with respect to the enthalpy of sublimation. Then, the one is relevant and is really responsible for the final calculated value.

Comparing data in Table 1, estimated using Eq.(2) for tetradecanol, pentadecanol, hexadecanol and octadecanol, it is clear the estimatives are highly cloded to the extrapolated data usind published data in NIST. Then, the Eq.(2) is really recommended and only the values estimated in the second methodwill be confirmed in the next topic of this work.

Melting points of ethers and esters proved to have a trend so far, see the work of Hasl and Jiricek, 2014 [47]. Similarly, the melting temperatures of alkanes within the carbon atomnumber range 8 – 20 are slightly similar, which is most likely due to the similar intensity of the intermolecular forces in the crystal lattice.

4. TESTING THE SOLID-LIQUID EQUILIBRIUM MODEL

Considering the complete equation for the solid‑liquid equilibrium (SLE) [28,29] published in Poling et al., 2001 and regarding that: (i) the triple point temperature is close to the melting temperature; (ii) the difference between the heat capacities of the liquid and solid phases is small; (iii) the contribution of enthalpy is higher than that of the heat capacity, and (iv) the solid phase can be considered as a pure component, the cited equation can be reduced to Eq. (5) described as follows:

$$\ln(x_i \gamma_i) = -\frac{\Delta H_{f,i}}{R}\left(\frac{T_{f,i}}{T} - 1\right. \tag{5}$$

Where xi is the mole fraction of component i, γi is the activity coefficient of i in the liquid phase, $\Delta H_{f,i}$_and Tf, i correspond to the melting enthalpy and temperature, T is the equilibrium temperature and R is the universal gas constant.

Note that the assumption of a pure solid phase is not valid in the extreme left of the diagrams, due to the existence of a solid solution. Howsoever, this region is quite small and its exact boundaries, in terms of molar fractions, are not yet well established.

In order to calculate the liquid phase activity coefficients theMargules-1-suffix model was used. The interaction parameter for the Margules-1-suffix was obtained by using the experimental activity coefficient at infinite dilution data, as the simple suggestion in this preliminar studying test.

Table 8 shows the relative deviation (RDX) for each experimental fusion enthalpy tested using the same data of activity coefficient model. The one-parameter obtained stayed between 3.12- 3.76.

Table8. *Influence of enthalpy of fusion chosen in the calculated water solubilitiy of 1-tetradecanol, 1-Pentadecanol, 1- Hexadecanol and 1-octadecanol.*

Compound.$_i$	ΔH_{pub}^{fus}	T$_f$ /K	$\gamma_{i,\infty}^{'298\,K}$	$x_{i,exp(**)}^{'298\,K}$	$x_{i,calc}^{'298\,K}$	RDX
1-tetradecanol	47.29	308.1	17.5*	0.00291	0.004255	0.467
	23.81	311.			0.013293	3.59
	22.01	311.6			0.014778	4.07
	49.37***	311.			0.003163	0.103
1-Pentadecanol	23.64	316.	18.78*	0.00175	0.010460	4.98
	54.73***	316.6			0.001515	0.131
	29.6	316.4			0.007150	3.085
	53.62***	316.9			0.001621	0.074
1- Hexadecanol	57.7***	80. - 370.	21.31*	0.000912	0.0007758[1]	0.149
	33.1	321.6			0.004055	3.45
	33.97	322.9			0.004056	3.45
1-octadecanol	40.1	330.3	23.38*	0.000225	0.0014472	5.43
	66.67***	331.2			0.0001830	0.187
	70.08	334.2			0.0001404	0.378

[1] considering fusion temperature of 321.6 K

$\gamma_{i,\infty}^{'298\,K}$- activity coefficient at infinite dilution of compound i in water at 298.15K published by Nanua et al., 2004[49].

$x_{i,exp(**)}^{298\,K}$- molar solubility of compound i in water published by Pinsuwan et al., 1997[48].

RDX = $\dfrac{x_{i,exp}^{298K} - x_{i,calc}^{298K}}{x_{i,exp}^{298K}}$ - Relative deviation

*** recommended by this work (Eq. 3)

The calculated solubility results for the systems1-tetradecanol, pentadecanol, hexadecanol and 1-octadecanol are also exibited in Table 8. Considering the small discrepancies among the results obtained from the first method, it was not necessary to take it into account here. For the second one, the best results achieved had the relative deviation shorter than 0.187. Clearly the results are linked to the model used and regarding that no further fitting is done to express thenon-ideality of the liquid phase.

Calculations based on the all fusion enthalpy data available provided very different solubilty results, showing that this thermo physical property had very strong influence in the solid-liquid equilibrium calculations.

Note that the last system corresponds to the alcohol molecule with higher carbon chain. In this case the association between the unlike molecules caused by the interaction between water molecules becomes more important and the mixture probably presents a stronger negative deviation from Raoult's law.

5. CONCLUSION

Quick estimations of ΔH_i^{fus}can be a profitable implement in the absence of published data due to the enthalpy of fusion available for alcohols are scarce and inconsistent. The predicted findings were compared with the published data, which are available from different authors. As it stands, it was feasible to choose the first or second method for predicting enthalpy of fusion. To confirm the second one, data predicted (ΔH_i^{fus}) was used in solid-liquid equilibrium calculations. Solubilities derived by solid-liquid equilibrium model were found in a good agreement with the experimental data when they were estimated using fusion enthalpy data recommended by the second method.

This not only makes sure that original equation continue to receive recognition for their application, it allows the workers to verify consistency with the reported data in the different sources and expert analysis of the quantified reliability of the information

This work presented the first attempt and needs to be improved in the future, since the one was restricted to alcohols compounds.

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