CHEMISTRY & CHEMICAL TECHNOLOGY

Vol. 10, No. 1, 2016 Chemistry

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CALCULATION METHOD OF HEAT CAPACITY CHANGE DURING ORGANIC COMPOUNDS VAPORIZATION AND SUBLIMATION

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Received: April 05, 2014 / Revised: June 04, 2014 / Accepted: September 02, 2014

Abstract. On the basis of literature data the constancy of heat capacity change during vaporization (± 2 %) and sublimation (± 8 %) has been determined at 298 K for different organic compounds. The obtained equations allow to recalculate the enthalpy according to Kirchhoff's law easier compared with present techniques based on the increments method. The vaporization and sublimation enthalpies of 5-(2-nitrophenyl)-furan-2-carbaldehyde have been determined and recalculated for 298 K for the reliability proofing of the suggested method.

Keywords: heat capacity, phase transition, enthalpy, sublimation, vaporization, 5-(2-nitrophenyl)-furan-2-carbaldehyde.

1. Introduction

Arylfurfurol derivatives are biologically active compounds. That is why they are used as the initial compounds during drugs synthesis [1]. The determination of their thermodynamic properties, namely sublimation and vaporization enthalpies, allows to solve some practical questions, optimize their purification and application, and extend the theoretical knowledge about their nature. Phase transfer enthalpies are determined by the experiments within the temperature range essentially differed from 298 K – the temperature at which they are represented in the reference books. Thus, the melting enthalpy is measured at the melting temperatures and the vaporization enthalpy is determined according to the temperature dependence of the saturated vapor pressure. The temperature ranges favorable for the investigations are various for different compounds and depend on their volatility. To recalculate these values for the standard ones it is necessary to know the heat capacity of the investigated compound under standard conditions.

The experimental measuring of heat capacity is very laborious and complicated method. Therefore the existing information about organic compounds heat capacity is very limited. Due to the same reason there are many attempts to solve the existing problem *via* empirical way, starting from the simplest one – calculation of the heat capacity relative to the atoms in the molecule and finishing by the modern method – relative to the increments [2, 3]. Such increments allow to calculate the heat capacity of some organic compounds in solid, liquid and gaseous states with the error of 7–10 %. Two suggested equations [3] allow to calculate the heat capacity change during vaporization (Eq. (1)) and sublimation (Eq. (2)) of the organic compounds:

$$(C_{p(l)} - C_{p(g)}) = 10.58 + 0.26 \cdot C_{p(l),298} \qquad (1)$$

$$(C_{p(s)} - C_{p(g)}) = 0.75 + 0.15 \cdot C_{p(s),298} \qquad (2)$$

where $C_{p(l,s,g),298}$ – heat capacity of the compound in liquid, solid or gaseous states, respectively, at 298 K.

The same characteristic during melting may be determined according to the difference between Eq. (2) and Eq. (1). In all cases the constants are determined relative to the increments typical of the examined molecule [3]. The given method has a series of shortcomings: the increment values are generalized and some of them are absent. These factors complicate the calculations, especially for the complex molecules.

The aim of this work is the search of more available method to calculate the above-mentioned values without using increments which are unknown for the majority of organic compounds. For this purpose we analyzed literature data containing information about heat capacity change during vaporization of different organic compounds at 298 K. To check the adequacy of obtained regularities and compliance with the existing methods we show the experimental results concerning the temperature dependence of saturated vapor pressure of 5-(2-nitrophenyl)-furan-2-carbaldehyde obtained *via* effusive method and recalculate the obtained values of enthalpies from the average temperatures to 298 K.

2. Experimental

2.1. Analysis of Heat Capacity Change at Phase Transitions

For the statistical calculations we used molar heat capacities of different organic compounds (aliphatic, alicyclic and aromatic hydrocarbons; alcohols; ketones; aldehydes; acids; nitrogen-, fluorine- and chlorine-containing compounds) in solid, liquid and gaseous aggregative states. These values were determined by different authors and published in the literature. Tables 1 and 2 represent the values of molar and specific heat capacity, as well as heat capacity change during vaporization (Table 1) and sublimation (Table 2). The standard deviation of the average value is calculated using the Student's coefficient (*t*-criterion) for the significance level of 0.95 [4].

The reason under which we analyzed the specific values of this thermodynamic characteristic instead of usual molar heat capacity is the following. Intermolecular forces are determinative in the processes of aggregative transformations and they are provided by all atoms in the molecule. Therefore their quantity in the mass (volume) unit is more important factor than the amount of molecules formed by them. Thus, at 298 K vaporization enthalpy of decane 1 mole is close to the enthalpy of pentane 2 moles. Actually, in the homologous series of normal alkanes (C_5–C_{17}) the specific vaporization enthalpies ($\Delta_{vap}H_{298}$) are almost the same (362 ± 2 J/g). The same situation but with other value (324 ± 6 J/g) is observed for branched 2,2-dimethylalkanes and 3,3,5,5-tetramethylalkanes. The similar examples may be continued. It is logically to assume that the heat capacity change which is the first derivative of enthalpy change will preserve such property. Thus, the standard value of heat capacity in the liquid state for methanol is 81.1 J/mol·K; for hexanol – 243.2 J/mol·K; the specific values of heat capacity are 2.53 and 2.38 J/g·K, respectively.

Table 1

Change of standard heat capacity during organic compounds vaporization at 298 K

Formula	Compound	MW, g/mol	$C_{p(l)}$, J/K		$C_{p(g)}$, J/K		$C_{p(g)} - C_{p(l)}$ J/g K
			/mol	/g	/mol	/g	
1	2	3	4	5	6	7	8
C_2H_4O	Ethanal	44.05	89.1 [5]	2.021	55.3 [5]	1.256	-0.765
C_4H_4O	Furan	68.07	114.6 [5]	1.683	64.4 [5]	0.946	-0.737
C_4H_6O	2,3-Dihydrofuran	70.09	121.1 [6]	1.728	72.3 [7]	1.031	-0.697
$C_4H_6O_2$	Butyrolacton	86.09	140.9 [8]	1.637	86.1 [9]	1.000	-0.637
$C_4H_6O_3$	4-Methyl-1,3-dioxolan-2-on	102.09	167.4 [5]	1.640	107.6 [5]	1.054	-0.586
C_4H_8	1-Butene	56.11	129.0 [10]	2.299	85.6 [11]	1.525	-0.774
$C_5H_4O_2$	Furfural	96.08	162.8 [13]	1.694	98.1[5]	1.021	-0.673
C_5H_7O	2-Methylfuran	82.10	143.7 [5]	1.751	89.7[5]	1.092	-0.659
C_5H_{10}	1-Pentene	70.13	154.9 [14]	2.209	108.2 [11]	1.543	-0.666
C_5H_{10}	Cyclopentane	70.13	126.7 [15]	1.807	82.8 [16]	1.181	-0.626
C_5H_{10}	Diethylketone	86.13	190.9 [5]	2.216	128.9 [17]	1.496	-0.720
C_5H_{10}	Methylpropylketone	86.13	185.4 [5]	2.152	121.0 [5]	1.405	-0.747
C_5H_{10}	Pentanal	86.13	174.4 [5]	2.025	122.6 [5]	1.423	-0.602
C_5H_{10}	*iso*-Propylmethylketone	86.13	179.9 [5]	2.089	122.8 [17]	1.425	-0.664
C_5H_{10}	Tetrahydrofuran	86.13	149.6 [18]	1.737	99.1 [19]	1.151	-0.586
C_5H_{12}	Pentane	72.15	167.2 [20]	2.317	120.1 [21]	1.664	-0.653
C_6H_6	Benzene	78.11	135.6 [22]	1.736	82.4 [11]	1.055	-0.681
C_6H_{12}	Cyclopentane-methyl	84.16	158.7 [23]	1.886	109.5 [11]	1.301	-0.585
C_6H_{12}	Cyclohexane	84.16	156.9 [22]	1.864	105.3 [16]	1.251	-0.613
$C_6H_{12}O$	*iso*-Butylmethylketone	100.16	211.9 [24]	2.116	147.5 [25]	1.473	-0.643
$C_6H_{12}O$	*tert*- Butylmethylketone	100.16	206.9 [5]	2.066	157.1 [25]	1.568	-0.498

Table 1 (Continued)

1	2	3	4	5	6	7	8
$C_6H_{12}O$	Hexanal	100.16	210.4 [26]	2.101	145.5 [27]	1.453	-0.648
$C_6H_{12}O$	Methylbutylketone	100.16	213.4 [28]	2.131	143.8 [5]	1.436	-0.695
$C_6H_{12}O$	Propylethylketone	100.16	216.9 [5]	2.166	151.0 [5]	1.508	-0.658
C_6H_{14}	Hexane	86.18	197.6 [29]	2.293	142.6 [27]	1.655	-0.638
C_7H_6O	Benzaldehyde	106.12	172.0 [5]	1.621	111.7 [5]	1.153	-0.568
C_7H_8O	Metoxybenzene	108.14	199.0 [30]	1.840	135.3 [5]	1.251	-0.589
C_7H_{14}	Methylcyclohexane	98.19	185.0 [15]	1.884	135.8 [11]	1.383	-0.501
C_7H_{14}	Cycloheptane	98.19	180.5 [31]	1.838	132.0[16]	1.344	-0.494
$C_7H_{14}O$	Heptanal	114.19	230.2 [5]	2.016	168.2[5]	1.473	-0.543
C_7H_{16}	Heptane	100.20	224.6 [32]	2.242	165.2 [33]	1.649	-0.593
C_7H_{16}	2-Methylhexane	100.20	222.9 [34]	2.225	165.4 [33]	1.651	-0.574
$C_7H_{16}O$	Heptanol	116.20	270.8 [5]	2.330	178.7 [5]	1.538	-0.792
C_8H_{10}	1,2-Dimethylbenzene	106.17	187.7 [35]	1.768	132.5 [36]	1.248	-0.520
C_8H_{10}	1,3-Dimethylbenzene	106.17	184.6 [37]	1.739	125.8 [36]	1.185	-0.554
C_8H_{10}	1,4- Dimethylbenzene	106.17	183.7 [38]	1.730	126.0 [12]	1.187	-0.543
$C_8H_{16}O$	Hexamethylketone	128.21	273.3 [5]	2.132	189.6 [5]	1.479	-0.653
$C_8H_{16}O$	Octanal	128.21	259.6 [5]	2.025	191.2 [5]	1.491	-0.534
C_8H_{18}	2-Methylheptane	114.23	252.0 [39]	2.206	187.2 [33]	1.639	-0.567
C_8H_{18}	Octane	114.23	255.7[40]	2.239	187.8 [33]	1.644	-0.595
C_8H_{18}	2,3,4-Trimethylpentane	114.23	247.3 [41]	2.165	191.6 [33]	1.677	-0.488
$C_8H_{18}O$	Octanol	130.23	304.0 [5]	2.334	201.5 [5]	1.548	-0.787
C_9H_{12}	Cumene	120.19	215.4 [42]	1.792	151.7 [27]	1.262	-0.530
C_9H_{12}	Propylbenzene	120.19	214.7 [43]	1.786	152.3 [27]	1.267	-0.519
C_9H_{12}	1,2,3-Trimethylbenzene	120.19	216.4 [44]	1.801	159.1 [45]	1.324	-0.477
C_9H_{12}	1,2,4- Trimethylbenzene	120.19	213.1 [46]	1.773	154.1 [45]	1.282	-0.491
C_9H_{12}	1,3,5- Trimethylbenzene	120.19	207.9 [37]	1.729	147.4[45]	1.226	-0.503
$C_9H_{18}O$	Nonanal	142.24	290.3 [5]	2.041	214.1 [5]	1.505	-0.536
C_9H_{20}	3,3-Diethylpentane	128.26	278.2 [47]	2.169	216.7 [33]	1.690	-0.479
C_9H_{20}	2,2,3,3,-Tetramethylpentane	128.26	271.5 [48]	2.117	212.1 [33]	1.654	-0.463
$C_{10}H_8$	Naphthalene	128.17	196.1 [49]	1.530	133.0 [11]	1.038	-0.492
$C_{10}H_{14}$	1,2,3,4-Tetramethylbenzene	134.22	244.3 [50]	1.820	186.1 [45]	1.387	-0.433
$C_{10}H_{14}$	1,2,3,5- Tetramethylbenzene	134.22	240.2 [51]	1.790	180.7 [45]	1.346	-0.444
$C_{10}H_{22}$	Decane	142.28	315.5 [40]	2.217	233.1[33]	1.638	-0.579
$C_{10}H_{20}O$	Decanal	156.27	319.7 [5]	2.046	237.0 [5]	1.517	-0.529
$C_{11}H_{10}$	1-Methylnaphthaline	142.20	224.4 [53]	1.578	159.3[11]	1.120	-0.458
$C_{12}H_{10}$	Diphenyl	154.21	259.5 [54]	1.683	166.7 [55]	1.081	-0.602
C_6H_7N	2-Methylpyridine	93.13	158.4 [56]	1.701	100.0 [27]	1.074	-0.627
C_6H_7N	3-Methylpyridine	93.13	158.7 [57]	1.704	99.6 [27]	1.070	-0.634
CH_3NO_2	Nitromethane	61.04	106.0 [58]	1.736	57.3[27]	0.939	-0.797
$C_2H_5NO_2$	Nitroethane	75.07	134.2 [59]	1.788	78.2 [27]	1.042	-0.746
$C_2H_4F_2$	1,1-Difluoroethane	66.05	118.4 [60]	1.793	67.9 [27]	1.028	-0.765
$C_6H_4F_2$	1,2-Difluorobenzene	114.09	159.0 [61]	1.394	106.5 [27]	0.933	-0.461
$C_6H_4F_2$	1,3-Difluorobenzene	114.09	159.1 [62]	1.395	106.3 [27]	0.932	-0.463
$C_6H_4F_2$	1,4-Difluorobenzene	114.09	159.1[63]	1.394	106.9 [27]	0.937	-0.457
C_6H_5F	Fluorobenzene	96.10	146.3 [64]	1.522	94.4 [27]	0.982	-0.540
$C_7H_5F_3$	Trifluoromethylbenzene	146.11	188.5 [65]	1.290	130.4 [27]	0.892	-0.398
C_7H_7F	1-Fluoro-4-methylbenzene	110.13	173.7 [66]	1.577	116.2 [27]	1.055	-0.522
C_6H_5Cl	Chlorobenzene	112.56	152.1 [67]	1.351	98.0 [27]	0.871	-0.480
Average value: -0.591 ± 0.024 J/g·K							

Table 2

Change of standard heat capacity during organic compounds vaporization at 298 K

Formula	Compound	MW, g/mol	$C_{p(l)}$, J/K		$C_{p(g)}$, J/K		$C_{p(g)} - C_{p(l)}$ J/g K
			/mol	/g	/mol	/g	
$C_2H_2O_4$	Oxalic acid	90.04	105.9 [5]	1.176	85.0 [57]	0.944	-0.232
$C_3H_4O_3$	1,3-Dioxolan-2-on	88.06	117.4 [5]	1.333	81.6 [5]	0.927	-0.406
$C_3H_6O_3$	1,3,5-Trioxane	90.08	111.4 [5]	1.237	82.4 [5]	0.915	-0.322
C_6H_6O	Phenol	94.11	127.45 [5]	1.354	103.2[5]	1.097	-0.257
$C_7H_6O_2$	Benzoic acid	122.12	146.8 [5]	1.202	103.5 [5]	0.847	-0.355
C_7H_8O	2-Methylphenol	108.14	154.6 [5]	1.429	127.3 [5]	1.177	-0.252
C_7H_8O	4-Methylphenol	108.14	150.3 [5]	1.389	125.0 [5]	1.156	-0.233
C_7H_{10}	2-Norborner	94.15	129.9 [68]	1.380	112.7 [69]	1.197	-0.183
$C_{10}H_8$	Naphthalene	128.17	165.7 [55]	1.293	133.0 [11]	1.038	-0.255
$C_{10}H_{14}$	1,2,4,5-Tetramethylbenzene	134.22	204.0 [52]	1.520	183.1 [45]	1.364	-0.156
$C_{11}H_{16}$	Pentamethylbenzene	148.25	270.3[52]	1.823	212.5 [45]	1.433	-0.390
$C_{12}H_{10}$	Diphenyl	154.21	198.4 [70]	1.287	166.7 [55]	1.081	-0.206
$C_{12}H_{12}$	1,8-Dimethylnaphthalene	156.22	241.8 [71]	1.548	189.2 [11]	1.211	-0.337
$C_{12}H_{12}$	2,3- Dimethylnaphthalene	156.22	216.5[71]	1.386	188.0 [11]	1.203	-0.183
$C_{12}H_{12}$	2,6- Dimethylnaphthalene	156.22	202.5 [71]	1.296	180.8 [11]	1.157	-0.139
$C_{12}H_{12}$	2,7- Dimethylnaphthalene	156.22	204.4 [71]	1.308	181.6 [11]	1.162	-0.146
$C_{13}H_{28}O$	1-Tridecanol	200.36	378.0 [72]	1.887	315.9[5]	1.577	-0.310
$C_{14}H_{28}O$	Tetradecanone	212.37	415.2 [73]	1.955	328.6 [5]	1.547	-0.408
$C_{14}H_{30}O$	1-Tetradecanol	214.39	426.5 [74]	1.989	338.7 [5]	1.580	-0.409
$C_{15}H_{30}O$	2-Pentadecanone	226.40	426.8 [73]	1.885	349.7 [5]	1.545	-0.340
$C_{15}H_{32}O$	1-Pentadecanol	228.41	400.0 [74]	1.751	361.6 [5]	1.583	-0.168
$C_{16}H_{34}O$	1-Hexadecanol	242.44	422.0 [74]	1.741	384.5 [5]	1.586	-0.155
$C_{18}H_{38}$	Octadecane	254.49	485.6 [75]	1.908	417.6 [27]	1.641	-0.267
C_6H_5Cl	Chlorbenzene	112.56	120.0 [76]	1.066	98.0 [27]	0.871	-0.195
$C_6H_4Cl_2$	1,4-Dichlorbenzene	147.00	147.8 [77]	1.005	113.9 [27]	0.775	-0.230
Average value: -0.261 ± 0.035 J/g·K							

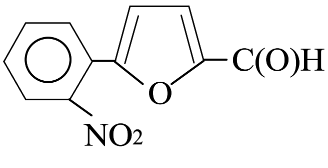
Table 3

Effusion investigations of 5-(2-nitrophenyl)-furan-2-carbaldehyde

Aggregative state	T, K	$\Delta m_{ef} \cdot 10^3$, g	$\tau \cdot 10^3$, s	p, Pa	T, K	$\Delta m_{ef} \cdot 10^3$, g	$\tau \cdot 10^3$, s	p, Pa
Solid	346.6	0.90	10.81	0.108	354.9	0.90	5.42	0.219
	347.9	0.80	9.02	0.116	358.6	1.45	5.41	0.355
	351.2	0.90	7.21	0.164	361.5	1.75	5.41	0.431
	351.2	0.95	7.22	0.173	363.1	1.55	3.62	0.572
	353.1	1.10	7.22	0.201	363.2	1.30	3.62	0.480
	353.2	0.60	3.62	0.218	368.0	2.46	3.62	0.913
	353.4	0.90	5.43	0.218	368.0	2.55	3.62	0.947
$\ln P = (34.2 \pm 1.8) - (12660 \pm 664) \cdot 1/T$; $\Delta H_{sub} = 105.3 \pm 5.2$ kJ/mol								
Liquid	378.0	6.60	3.62	2.484	387.9	6.00	1.82	4.561
	378.0	6.60	3.62	2.485	388.5	5.90	1.83	4.464
	382.7	4.45	1.83	3.342	389.7	6.50	1.82	4.950
	383.0	9.00	3.62	3.410	393.0	7.75	1.82	5.914
	386.6	5.25	1.82	3.980	393.3	7.75	1.82	5.933
$\ln P = (23.2 \pm 1.0) - (8420 \pm 404) \cdot 1/T$; $\Delta H_{vap} = 70.0 \pm 2.4$ kJ/mol								

2.2. Synthesis, Confirmation of Identity and Determination of Saturated Vapor Pressure for 5-(2-Nitrophenyl)-furan-2-carbaldehyde

Under normal conditions 5-(2-nitrophenyl)-furan-2-carbaldehyde is a crystalline substance with the melting temperature $T_m = 368.3 \pm 1.0$ K (determined by a capillary method):



The investigated compound was obtained *via* interaction between furfural and arendiazonium chloride obtained by diazotation of 2-nitroaniline. The obtained precipitate was filtered and purified by multifold recrystallization in the mixture with ethanol dimethylformamide. The compound identity was confirmed by NMR-spectroscopy using Varian 600 (600 MHz) instrument and DMSO-*d*6 solvent. The chemical shifts (*d*, ppm) were recorded relative to DMSO signal (2.5 ppm). ^{1}H NMR (600 MHz, DMSO) δ 7.24 (d, J = 3.7 Hz, 1H, fur), 7.72 (d, J = 3.7 Hz, 1H, fur), 7.79 (t, J = 7.8, 1H, C_6H_4), 7.88 (t, J = 7.8 Hz, 1H, C_6H_4), 7.99 (d, J = 7.8, 1H, C_6H_4), 8.07 (d, J = 7.8 Hz, 1H, C_6H_4), 9.66 (s, 1H, CHO).

Temperature dependence of the saturated vapor pressure, as well as sublimation and vaporization enthalpies were determined *via* Knudsen integral effusion method. The experimental plant and its reliability test are described in Ref. [78]. The weight of effunded compound (Δm_{ef}) was determined by weightening of the effusion chamber with the accuracy of $\pm 5 \cdot 10^{-5}$ g. The accuracy of temperature (T) and effusion time (t) measurements was ± 0.1 K and ± 10 s, respectively. The hole diameter in membrane and its thickness were 0.591 and 0.050 m, respectively. The results of effusion measurements including the saturated vapor pressure (p), linear equation of temperature dependence of the saturated vapor pressure within the coordinates of the Clausius-Clapeyron equation and heat of the corresponding phase transitions are represented in Table 3.

3. Results and Discussion

While analyzing the standard heat capacities of the compounds in solid, liquid and gaseous states (Tables 1 and 2) we used the general procedure of statistical selection. At first we declined 12 compounds from 81 ones for the vaporization process (Table 2) and 4 compounds from 29 ones for the sublimation process (Table 3) because their characteristics differ from the average values by more than $\pm 2s$. At the second stage we analyzed the possible existence of the heat capacity change dependence during vaporization of different organic compounds. Alcohols and nitrocompounds have the value that is higher than the average one $C_{p(g)} - C_{p(l)} = 0.78$ J/g·K; aromatic, fluorine- and chlorine-derived compounds have a lower value (0.49 J/g·K). It should be also noted that the number of analyzed compounds sometimes was miserable: *e.g.* for alcohols – 3; for nitrocompounds – 2; for fluorine-derived – 5 and for chlorine-derived – 2. The analysis using *t*-criterion confirms that these samples are statistically indistinguishable and may be treated as one generalized sample with average values and dispersions given below in Eqs. (3) and (4).

The results of statistical analysis show the consistency of heat capacity change during vaporization and sublimation at 298 K (Tables 1 and 2), according to which the molar heat capacity change may be determined according to the following equations:

$$\Delta_{vap}C^0_{p_{298}} = (C_{p(g)} - C_{p(l)}) = -(0.591 \pm 0.024) \cdot M \qquad (3)$$

$$\Delta_{sub}C^0_{p_{298}} = (C_{p(g)} - C_{p(c)}) = -(0.261 \pm 0.035) \cdot M \qquad (4)$$

To check the suggested equations we recalculated the experimental values of sublimation and vaporization enthalpies obtained within *p–T* range for 298 K using the Kirchhoff's equation and then compared them.

$$\Delta H_{298} = \Delta H_T - \int_{298}^{T} \Delta C_p dT$$

where ΔH_T – enthalpy of phase transition determined at the average temperature of investigated *p–T* interval; ΔC_p – heat capacity change at phase transition

For the comparison we used sublimation and vaporization enthalpies determined by the calorimetric method using reference substances at 298 K (Table 4) and vaporization enthalpies obtained by *p–T* measurements and recalculated using the Kirchhoff's equation and known values of heat capacity in condensed and gaseous states at 298 K.

Vaporization enthalpies of nonane, decane, decanol-1 and 1,4-dimethylbenzene, as well as sublimation enthalpies of benzoic acid and bicycle[2,2,2]octane were obtained by the calorimetric method at 298 K. It is impossible to determine the sublimation enthalpies of nonane, decane, and decanol-1 at 298 K because their melting temperatures are lower than the mentioned one. The given values were calculated using sublimation values obtained by the experiments and recalculated to the standard values using heat capacities of the compounds in solid and gaseous states.

Table 4

Comparison of vaporization enthalpies at 298 K calculated by known equations (1) and (2) and suggested ones (3) and (4) with experimental values

Compound	$\Delta_{vap}H_{298}$, kJ/mol			$\Delta_{sub}H_{298}$, kJ/mol		
	Exp.	Eq., according to which ΔC_p is calcl.		Exp.	Eq., according to which ΔC_p is calcl.	
		(1)	(3)		(2)	(4)
Nonane	46.43 [79]	47.8	46.5	71.4 [80]	71.4	71.9
Decane	51.4±0.1 [79]	52.9	51.3	82.4 [80]	82.4	82.8
Decanol-1	81.5±0.8 [3]	80.4	80.5	112.5±6.3 [81]	114.3	114.3
Benzoic acid				89.5±1.8 [82]	88.4	88.7
Bicyclo[2,2,2]octane				48±2[83]		47.6
1,4-Dimethylbenzene	42.4±0.1 [3]	43.1	42.8			
5-(2-Nitrophenyl)-furan-2-carbaldehyde	–	78.2	80.8	–	107.8	108.2

While comparing the experimental values calculated in accordance with known Eqs. (1) and (2) and suggested ones (3) and (4) we observe the similarity of the obtained results; the difference is within experimental and calculation errors. Table 4 also represents the comparison of enthalpies of the investigated aldehyde recalculated by different methods.

Taking into account all mentioned above, one can see that the known complicated calculation methods have no essential advantages compared with the simpler method suggested by us.

4. Conclusions

The recalculation of vaporization and sublimation enthalpies for 298 K using the suggested simple equations allows to obtain the results with the error of 2–8 %. It is tantamount to the application of existed additive methods based on increments principle. Vaporization and sublimation enthalpies of 5-(2-nitrophenyl)-furan-2-carbaldehyde were experimentally determined within the temperature range when the compound is in solid and liquid aggregative states. The adequacy of proposed method with the existing calculations is confirmed. The suggested Eqs. (3) and (4) have only empirical character. Therefore their application while extrapolation calculations for the compounds with the molecular weight over 250 g/mol and phase transition temperature over 550 K is limited.

Acknowledgments

The author thanks Dr. Y.Horak for the given sample of 5-(2-nitrophenyl)-furan-2-carbaldehyde and post-graduated students A. Marshalek and M. Punyak for their assistance during effusive investigations.

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МЕТОД РОЗРАХУНКУ ЗМІНИ ТЕПЛОЄМНОСТІ ПРИ ВИПАРОВУВАННІ ТА СУБЛІМАЦІЇ ОРГАНІЧНИХ СПОЛУК

Анотація. *За результатами аналізу джерел літератури встановлено постійність зміни теплоємності за 298К при випаровуванні (±2 %) та сублімації (±8 %) органічних сполук різних класів. Одержані рівняння дають можливість проводити простіший перерахунок ентальпій за рівнянням Кірхгофа порівняно з існуючими методами, побудованими за принципом групових внесків. Для перевірки надійності запропонованого метода вперше визначено ентальпії випаровування та сублімації 5-(2-нітрофеніл)-фуран-2-карбальдегіда та проведено відповідні перерахунки на 298 К.*

Ключові слова: *теплоємність фазових переходів, ентальпії сублімації та випаровування, 5-(2-нітрофеніл)-фуран-2-карбальдегід.*