

Vaporization enthalpies of a series of the fluoro- and chloro-substituted methylbenzenes

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ABSTRACT

Vapor pressures of fluorobenzene, chlorobenzene, 2-chloro-, 3-chloro-, and 4-chloro-methylbenzenes, 2-chloro-1,3-dimethylbenzene, 2,6-dichloro-1-methylbenzene were measured by the transpiration method. Molar standard enthalpies of vaporization at the reference temperature were calculated from temperature dependences of vapor pressures. Available literature data on halogenobenzenes were collected and evaluated by using correlation gas-chromatographic method. Simple group-additivity procedure was developed for estimation vaporization enthalpies of mono- and di-halogen-substituted benzenes.

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1. Introduction

Halogen substituted benzenes belong to the long-lived pollutants frequently found in industrial effluents. Reliable thermodynamic data for these compounds are of an environmental interest [1]. Careful search for primary experimental data on halogenobenzenes available in literature has been performed in this work. It has turned out that the good quality primary vapor pressures and vaporization enthalpies exist only for fluorobenzene and chlorobenzene (see Table 1). Collection of experimental data available for fluoro- and chloro-substituted methylbenzenes suffered from ambiguity. Indeed, the comprehensive compilations by Stull [2] and by Stephenson and Malanowski [3] contain vapor pressure data for numerous halogen substituted benzenes over a wide range of temperature. The origin of the data presented there is not clear, methods of measurements are unknown, as well as errors of measurements and purities of compounds. In this context, additional measurements on halogen substituted methylbenzenes are desired. As a part of our systematic research on thermochemical properties of halogen organic compounds [4–6] this paper

presents new vapor pressure data for seven halogen substituted benzenes and methylbenzenes: fluorobenzene, chlorobenzene, 2-chloro-, 3-chloro-, and 4-chloro-methylbenzenes, 2-chloro-1,3-dimethylbenzene, 2,6-dichloro-1-methylbenzene. Molar standard enthalpies of vaporization, $\Delta_1^g H_m$, for these compounds were calculated from temperature dependences of vapor pressures. We also collected vapor pressures of halo-methylbenzenes available in the literature and treated these data uniformly in order to derive and evaluate their enthalpies of vaporization. The evaluated values of $\Delta_1^g H_m$ (298.15 K) were used to develop a group-additivity procedure for mono- and di-halogen-substituted benzenes.

2. Experimental

2.1. Materials

The samples used for the transpiration experiments were of commercial origin. Origin of samples and initial purity are given in Table 1. Prior to experiments the samples were purified by repeated vacuum fractional distillation with the Teflon spinning-band column under reduced pressure. The final degree of sample purity was determined by using a Hewlett Packard gas chromatograph 5890 Series II equipped with a flame ionization detector and a Hewlett Packard 3390A integrator. The carrier gas (nitrogen)

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List of symbols

$\Delta_1^g H_m$	molar enthalpy of vaporization
T_a	ambient temperature
p_i	vapor pressure
C_p^l	molar heat capacities of liquid at constant pressure
C_p^g	molar heat capacities of gas at constant pressure
$\Delta_1^g C_p$	difference of the molar heat capacities at constant pressure

flow was $12.1 \text{ cm}^3 \text{ s}^{-1}$. A capillary column HP-5 (stationary phase crosslinked 5% phenyl methyl silicone) was used with a column length of 30 m, an inside diameter of 0.32 mm, and a film thickness of 0.25 μm . The standard temperature program of the GC was $T = 333.15 \text{ K}$ for 180 s followed by a heating rate of 0.167 K s^{-1} to $T = 523.15 \text{ K}$. No impurities (greater than mass fraction 0.002) could be detected in the samples used for the thermochemical measurements (see Table 2).

2.2. Vapor pressure measurements

Vapor pressures of halogen benzenes were determined using the method of transpiration [7,8] in a saturated nitrogen stream. About 0.5 g of the sample was mixed with small glass beads and placed in a thermostatted U-shaped saturator. A well defined nitrogen stream was passed through the saturator at a constant temperature ($\pm 0.1 \text{ K}$), and the transported material was collected in a cold trap. The amount of condensed sample was determined by GC analysis using an appropriate external standard ($n\text{-C}_n\text{H}_{2n+2}$). The absolute vapor pressure p_i at each temperature T_i was calculated from the amount of the product collected within a definite period of time. Assuming validity of the Dalton's law applied to the nitrogen stream saturated with the substance i , values of p_i were calculated with equation:

$$p_i = \frac{m_i \times R \times T_a}{V \times M_i}; \quad V = V_{\text{N}_2} + V_i; \quad (V_{\text{N}_2} \gg V_i) \quad (1)$$

where $R = 8.314472 \text{ J K}^{-1} \text{ mol}^{-1}$; m_i is the mass of the transported compound, M_i is the molar mass of the compound, and V_i is volume contribution to the gaseous phase. V_{N_2} is the volume of the carrier gas and T_a is the temperature of the soap bubble meter used for measurement of the gas flow. The volume of the carrier gas V_{N_2} was determined from the flow rate and the time measurement.

3. Results and discussion

3.1. Vapor pressure and vaporization enthalpies

Vapor pressures of halogenobenzenes measured at different temperatures were fitted with the following equation [8]:

$$R \times \ln p_i = a + \frac{b}{T} + \Delta_1^g C_p \times \ln \left(\frac{T}{T_0} \right), \quad (2)$$

where a and b are adjustable parameters and $\Delta_1^g C_p$ is the difference of the molar heat capacities of the gaseous and the liquid phase, respectively. T_0 appearing in Eq. (2) is an arbitrarily chosen reference temperature (which has been chosen to be 298.15 K). Consequently, vaporization enthalpy at temperature T was indirectly derived from the temperature dependence of vapor pressures using following equation:

$$\Delta_1^g H_m(T) = -b + \Delta_1^g C_p \times T \quad (3)$$

Values of $\Delta_1^g C_p$ have been calculated according to the procedure developed by Chickos et al. [9] based on isobaric molar heat

capacities C_p^l available in the literature (see Table S1, ESI). In case the C_p^l values were absent, we estimated them by a group-contribution method [10]. Experimental results for halobenzenes and parameters a and b are listed in Table 3.

The compilation of vaporization enthalpies for halobenzenes from this work and from the literature is presented in Table 1. Temperature dependencies of vapor pressures of halobenzenes have been reported numerous times. However, authors have not always calculated enthalpies of vaporization from their results. We collected and systematically treated experimental literature data using Eqs. (2) and (3) with $\Delta_1^g C_p$ -values listed in Table S1, ESI and calculated $\Delta_1^g H_m$ (298.15 K) for the sake of comparison with our results as well as for the evaluation of the data aiming the recommendation of vaporization enthalpies $\Delta_1^g H_m$ (298.15 K) for further thermochemical calculations.

3.1.1. Vaporization enthalpies of fluorobenzene and chlorobenzene

A very consistent set of vaporization enthalpies measured directly (calorimetric) and indirectly (from vapor pressure temperature dependence) was found for both fluorobenzene and chlorobenzene (see Table 1). Our own transpiration method measurements on these compounds were performed rather to in order to collect experimental experiences and possible peculiarities working with these volatile type of compounds. Our own $\Delta_1^g H_m$ (298.15 K) results for fluorobenzene and chlorobenzene were in very good agreement with those from the most reliable calorimetric, static, and ebulliometric methods (see Table 1). Such a good agreement has validated using of the transpiration method for the reliable determination of vaporization enthalpies of similar shaped halogen substituted methylbenzenes, where the available experimental data were found to be less consistent.

3.1.2. Vaporization enthalpies of fluoro-methylbenzenes

Most of the vapor pressure data available for fluoro-methylbenzenes were measured by static methods [15–17]. Enthalpies of vaporization, $\Delta_1^g H_m$ (298.15 K), derived from these vapor pressures by using Eq. (3) are presented in Table 1. As can be seen, enthalpies of vaporization of 2-, 3-, and 4-methyl-fluorobenzenes were hardly distinguishable within their boundaries of experimental uncertainties. They were randomly distributed around the value of 39 kJ mol^{-1} . There were at least 2–3 vapor pressure data sets with the traceable origin for each methyl-fluorobenzene. Results from vapor pressures compilations [2,3] were also in close agreement with those from the static [15–17] and ebulliometric measurements [18]. Having established such a consistent set on vaporization enthalpies for 2-, 3-, and 4-methyl-fluorobenzenes, no additional experimental studies were performed with these compounds.

3.1.3. Vaporization enthalpies of chloro-methylbenzenes

The very first experimental vaporization enthalpies of 2- and 4-chloro-methylbenzenes were reported already in 1926 by using the direct calorimetric method [40]. However the experimental values were measured at elevated temperatures around 430 K and were not adjusted to the reference temperature 298.15 K. In 1940 vapor pressures of all three chloro-methylbenzenes were measured in the range 277–348 K by the static method devised by Ramsay and Young [44]. The data were only fitted to suitable equations and vaporization enthalpies were not derived. The most recent vapor pressure data on 2- and 4-chloro-methylbenzenes were reported in 1982 from ebulliometric measurements at elevated temperatures close to the normal boiling point [42]. In this work we derived enthalpies of vaporization, $\Delta_1^g H_m$ (298.15 K), from data available in the literature (see Table 1). In addition we

Table 1
Compilation of data on enthalpies of vaporization, $\Delta_1^g H_m$, of the halobenzenes.

Compounds	Technique ^a	T-range/K	$\Delta_1^g H_m(T_{av})/kJ\ mol^{-1}$	$\Delta_1^g H_m(298.15\ K)^b/kJ\ mol^{-1}$	Ref.
Fluorobenzene	n/a	229.8–357.9	35.3	34.62 ± 0.08	[2]
	C	318.0–382.0	31.2	34.68 ± 0.10	[11]
	S	255.3–357.0	34.7	34.64 ± 0.06	[12]
	Eb	312.6–393.7	32.9	35.38 ± 0.05	[13]
	Eb	313.2–353.2	33.5	35.17 ± 0.05	[14]
	n/a	358–530	30.5	37.6 ± 3.0	[3]
	n/a	373–419	31.6	36.4 ± 3.0	[3]
	n/a	414–501	30.7	38.4 ± 3.0	[3]
	n/a	497–561	31.3	42.5 ± 5.0	[3]
	T	274.2–303.2	35.1	34.52 ± 0.23	This work
			35.01 ± 0.30	Average	
2-Fluoro-methyl-benzene	n/a	249.0–387.2	38.3	38.9 ± 2.0	[3]
	S	308.2–343.2	37.8	39.26 ± 0.40	[15]
	n/a	295–388	37.2	39.6 ± 3.0	[3]
	S	452.9–530.4	31.7	42.4 ± 3.0	[16]
	S	285.0–387.5	37.7	39.5 ± 2.0	[17]
			39.31 ± 0.38	Average	
3-Fluoro-methyl-benzene	n/a	250.8–389.2	38.7	39.4 ± 2.0	[2]
	S	308.2	37.4	38.95 ± 0.31	[15]
	S	293–390	37.6	40.0 ± 3.0	[3]
	S	285.0–389.7	38.1	39.9 ± 2.0	[17]
			38.99 ± 0.30	Average	
4-Fluoro-methyl-benzene	C	298.2–389.2		39.47 ± 0.10	[11]
	n/a	251.4–390.2	38.8	39.6 ± 2.0	[2]
	S	308.2–343.2	36.3	37.81 ± 0.32	[15]
	E	340.8–428.4	36.1	40.78 ± 0.07	[18]
	n/a			39.41 ± 0.08	[19]
S	285.0–389.7	38.0	39.9 ± 2.0	[17]	
			39.98 ± 0.30	Average	
Chlorobenzene	E	335.2–404.9	38.0	41.62 ± 0.03	[20]
	E	404.6–462.1	36.9	43.80 ± 0.06	[21]
	E	320.6–404.8	38.0	41.27 ± 0.54	[22]
	E	328.2–353.2	39.6	41.74 ± 0.73	[14]
	T	259.0–313.2	48.1	(47.36 ± 0.94)	[23]
	S	298.2–398.2	39.0	41.28 ± 0.71	[24]
	S	313.2–393.2	39.0	41.18 ± 0.06	[25]
	S	293.2–393.2	39.2	41.18 ± 0.16	[26]
	E	371.8–403.7	35.3	39.72 ± 0.64	[27]
	E	373.5–404.8	37.3	41.89 ± 2.0	[28]
	S	298.0–398.1	38.6	40.82 ± 0.35	[29]
	E	298.2–318.5	40.9	41.44 ± 0.27	[30]
	E	353.2–368.2	39.3	42.5 ± 2.0	[31]
	n/a	405.2–597.2	35.0	45.3 ± 5.0	[32]
	n/a	333–405	38.0	41.6 ± 3.0	[3]
	n/a	405–597	34.8	45.0 ± 5.0	[3]
	n/a	260.2–405.4	40.0	41.3 ± 2.0	[2]
	n/a	228.0–632.4	38.7	42.28 ± 0.35	[33]
	E	372.4–452.5	36.7	42.36 ± 0.08	[34]
		238.1–258.1	42.3	39.74 ± 0.40	[35]
	343.2–405.4	38.1	41.92 ± 0.15	[36]	
	293.2–353.2	40.2	41.32 ± 0.08	[37]	
n/a	329.4–404.9	38.1	41.44 ± 0.07	[38]	
C	298.15	–	40.97 ± 0.06	[39]	
C	403.7	36.6	41.89 ± 0.04	[40]	
S	303.1–405.1	38.8	41.41 ± 0.13	[41]	
T	274.5–307.2	41.7	41.22 ± 0.27	This work	
			41.76 ± 0.30	Average	
2-Chloro-methyl-benzene	E	345.8–431.5	41.3	46.39 ± 0.09	[42]
	n/a	338.0–493.0	40.1	46.7 ± 3.0	[3]
	n/a	293.2–433.2	42.6	45.8 ± 2.0	[43]
	C	431.2	38.5	46.07 ± 0.05	[40]
	S	277.0–348.0	44.8	45.5 ± 2.0	[44]
	n/a	278.5–432.4	43.0	45.7 ± 3.0	[2]
T	274.2–306.2	47.0	46.44 ± 0.40	This work	
			46.14 ± 0.30	Average	
3-Chloro-methyl-benzene	S	277–348	45.4	46.1 ± 2.0	[44]
	n/a	277.9–435.4	42.2	44.8 ± 3.0	[2]
	T	274.2–309.2	47.4	46.94 ± 0.49	This work
			46.84 ± 0.37	Average	
4-Chloro-methyl-benzene	C	433.5	38.7	46.35 ± 0.02	[40]
	E	338.0–433.0	42.0	46.86 ± 0.05	[42]
	n/a	293.2–423.2	42.3	45.3 ± 2.0	[43]
	S	277–348	45.3	46.0 ± 2.0	[44]
	n/a	278.6–435.4	42.5	45.2 ± 3.0	[2]
	n/a	304–436	41.2	45.2 ± 3.0	[3]
T	274.3–309.2	47.0	46.50 ± 0.33	This work	

Table 1 (Continued)

Compounds	Technique ^a	T-range/K	$\Delta_1^g H_m(T_{av})/kJ\ mol^{-1}$	$\Delta_1^g H_m(298.15\ K)^b/kJ\ mol^{-1}$	Ref.
2,6-Dichloro-1-methylbenzene	T	274.5–305.4	50.4	46.42 ± 0.30 49.78 ± 0.33 50.2	Average This work Additivity
1,3-Dichloro-2-methylbenzene	T	274.2–305.3	52.2	51.60 ± 0.29 52.4	This work Additivity
2,4-Dichloro-1-methylbenzene	n/a n/a	293–433 346–475	52.0 46.3	55.6 ± 2.0 53.5 ± 3.0 52.4	[43] [3] Additivity
3,4-Dichloro-1-methylbenzene	n/a	378–543	46.0	56.5 ± 3.0 52.4	[3] Additivity
2,5-Dichloro-1,4-dimethylbenzene	n/a	393–573	49.0	62.3 ± 3.0 56.6	[3] Additivity

^a Techniques: C = calorimetry; E = ebulliometry; S = static method; T = transpiration method.

^b Uncertainties are expressed as the standard deviation. Values in brackets were not taken into account.

performed own transpiration measurements on all three chloro-methylbenzenes in the low temperature range in order to get vaporization enthalpies possibly close to the reference temperature 298.15 K. Similar to fluoro-methylbenzenes, vaporization enthalpies of 2-, 3-, and 4-chloro-methylbenzenes measured by us were also indistinguishable (around of 46 kJ mol⁻¹) within their boundaries of experimental uncertainties.

3.1.4. Vaporization enthalpies of chloro-dimethylbenzenes and dichloro-methylbenzenes

In contrast to the very consistent vaporization enthalpies discussed for fluoro- and chloro-methylbenzenes the data available for chloro-dimethylbenzenes and dichloro-methylbenzenes are scarce and less reliable. Most of the collected vapor pressure data sets (see Table 1) of ambiguous quality were taken from the compilation [3]. In order to contribute to this kind of substitution and evaluate the available data we measured enthalpies of vaporization of 1-chloro-2,6-dimethylbenzene and 1,3-dichloro-2-methylbenzene using the transpiration method (see Tables 1 and 3). In general there was a lack of literature data on poly-methyl and poly-halogen benzenes available for comparison. For this reason we were encouraged to develop some correlation methods in order to evaluate consistency of the experimental data collected in Table 1.

3.2. Evaluation of vaporization enthalpies $\Delta_1^g H_m(298.15\ K)$ of halobenzenes

Correlation of experimental vaporization enthalpies with the structure related parameters is a valuable tool for the data evaluation. For example, vaporization enthalpies $\Delta_1^g H_m(298.15\ K)$ exhibit a good linear function of the number of carbon atoms in the chain of the *n*-alkanes [45] or *n*-alkyl-nitriles [46]. Linear correlations of $\Delta_1^g H_m(298.15\ K)$ of the geminal substituted azides [47] or aromatic ethers [48] with the data for similar structured molecules help to evaluate the experimental data. Both these

methods fail to be applied to the benzene derivatives. However, there are some useful correlations of vaporization enthalpies with the gas-chromatographic parameters such as Kovat's index [49], or temperature dependences of the retention times. We used both methods in the past to assess consistency of vaporization enthalpies measured for ethers [50], esters [51], and aldehydes [52] successfully.

3.2.1. Correlation of vaporization enthalpies $\Delta_1^g H_m(298.15\ K)$ of halobenzenes with Kovat's indices

Gas-liquid chromatography is widely used for non-analytic applications. The main measurable value in this method is the retention time of the analyte. Most frequently the retention time is recalculated into the more universal Kovat's index. Compilations of Kovat's indices are very useful for the content identification in different natural and synthetic mixtures [49]. The correlation of the enthalpies of vaporization with the Kovat's indices helps to reveal structure-property relations within series of parent compounds [51,53]. Indeed, we have already noticed above, that evaluated enthalpies of vaporization of 2-, 3-, and 4-fluoro-methylbenzenes were indistinguishable within their boundaries of experimental uncertainties (see Table 1). It has turned out that Kovat's indices measured for these isomers on the squalane packed column at 373 K [54] were also indistinguishable. The same observation was made for the Kovat's indices of all three fluoro-methylbenzenes measured (see Table S2, ESI) with the methyl silicone capillary column [55]. These facts have proved an inherent qualitative relationship between vaporization enthalpies and Kovat's indices. Similar conclusion was apparent for the chloro-substituted species: their very close enthalpies of vaporization measured in this work for 2-, 3-, and 4-methyl-chlorobenzenes (see Tables 1 and 2) were also in accordance with the very close Kovat's indices (952, 960, and 958) measured for these solutes with a E-301 capillary column at 373 K [56].

Having established the inherent qualitative relationship between vaporization enthalpies and Kovat's indices it has been

Table 2
Provenance and purity of the materials.

Material	CASRN	Origin	GC purity (mass fraction) ^a
Fluorobenzene	462-06-6	Sigma-Aldrich, 99%	0.999
Chlorobenzene	108-90-7	Sigma-Aldrich, 99.8%	0.999
2-Chloro-methylbenzene	95-49-8	Sigma-Aldrich, 99%	0.999
3-Chloro-methylbenzene	108-41-8	Sigma-Aldrich, 99%	0.998
4-Chloro-methylbenzene	106-43-4	Sigma-Aldrich, 99%	0.999
1-Chloro-2,6-dimethyl-benzene	6781-98-2	Alfa Aesar, 98%	0.998
1,3-Dichloro-2-methylbenzene	118-69-4	Sigma-Aldrich, 99%	0.999

^a Purity after fractional distillation under reduced pressure.

Table 3Results from measurements of the vapor pressure p of fluoro- and chloro-methylbenzenes using the transpiration method.

T^a (K)	m^b (mg)	$V_{(N_2)}^c$ (dm ³)	Gas-flow (dm ³ h ⁻¹)	p^d (Pa)	$(p_{exp}-p_{calc})^e$ (Pa)	$\Delta_1^g H_m$ (kJ mol ⁻¹)
Fluorobenzene; $\Delta_1^g H_m$ (298.15 K) = (34.52 ± 0.23) kJ mol ⁻¹ $\ln(p/\text{Pa}) = \frac{241.11}{R} - \frac{49,006.63}{R \times (T, K)} - \frac{48.6}{R} \ln\left(\frac{T, K}{298.15}\right)$						
274.2	8.20	0.082	0.98	2982.9	32.5	35.68
278.2	10.31	0.082	0.98	3644.8	-48.1	35.49
283.2	14.12	0.082	0.98	4836.3	-1.6	35.25
288.2	18.66	0.082	0.98	6259.5	-7.9	35.00
293.2	24.29	0.082	0.98	8024.7	-9.4	34.76
298.2	31.50	0.082	0.98	10,286.4	90.1	34.52
303.2	39.42	0.082	0.98	12,768.7	-49.6	34.27
Chlorobenzene; $\Delta_1^g H_m$ (298.15 K) = (41.22 ± 0.27) kJ mol ⁻¹ $\ln(p/\text{Pa}) = \frac{250.06}{R} - \frac{56,306.38}{R \times (T, K)} - \frac{50.6}{R} \ln\left(\frac{T, K}{298.15}\right)$						
274.5	9.67	0.635	2.54	367.9	1.4	42.42
277.3	11.10	0.593	2.54	444.2	2.2	42.28
280.3	12.52	0.550	2.54	532.2	-5.5	42.13
283.3	14.30	0.508	2.54	650.2	-0.7	41.97
286.3	16.15	0.466	2.54	793.0	8.6	41.82
289.3	17.72	0.423	2.54	949.7	8.7	41.67
292.2	18.93	0.381	2.54	1120.7	3.5	41.52
295.2	19.64	0.339	2.54	1302.4	-26.4	41.37
298.2	20.35	0.296	2.54	1535.9	-38.0	41.22
301.2	21.35	0.254	2.54	1871.8	14.9	41.07
304.2	20.67	0.212	2.54	2169.4	-13.0	40.92
307.2	19.96	0.169	2.54	2611.0	55.8	40.76
2-Chloro-methylbenzene; $\Delta_1^g H_m$ (298.15 K) = (46.44 ± 0.40) kJ mol ⁻¹ $\ln(p/\text{Pa}) = \frac{263.50}{R} - \frac{63,408.82}{R \times (T, K)} - \frac{56.9}{R} \ln\left(\frac{T, K}{298.15}\right)$						
274.2	3.39	0.820	1.41	86.42	1.02	47.81
277.1	3.90	0.750	1.41	107.2	0.9	47.64
280.3	3.86	0.586	1.41	134.2	-0.4	47.46
283.2	5.07	0.644	1.41	159.2	-6.6	47.30
286.1	4.45	0.434	1.41	205.8	2.7	47.13
288.2	5.76	0.504	1.41	228.3	-6.3	47.01
291.2	6.26	0.422	1.41	294.4	7.3	46.84
294.1	6.70	0.375	1.41	353.2	5.9	46.68
297.2	6.12	0.281	1.41	429.5	5.7	46.50
297.2	5.54	0.258	1.41	424.0	0.2	46.50
297.2	6.60	0.305	1.41	427.3	3.6	46.50
300.2	5.31	0.211	1.41	495.7	-15.6	46.33
303.2	3.68	0.117	1.41	616.5	2.3	46.16
306.2	4.39	0.117	1.41	734.9	0.2	45.99
3-Chloro-methylbenzene; $\Delta_1^g H_m$ (298.15 K) = (46.94 ± 0.49) kJ mol ⁻¹ $\ln(p/\text{Pa}) = \frac{262.70}{R} - \frac{63,397.25}{R \times (T, K)} - \frac{55.2}{R} \ln\left(\frac{T, K}{298.15}\right)$						
274.2	3.83	1.003	1.50	79.75	3.07	48.26
277.2	4.70	0.978	1.50	98.96	2.56	48.10
280.2	4.54	0.777	1.50	119.0	-1.5	47.93
283.1	3.84	0.539	1.50	144.0	-4.7	47.77
286.2	4.70	0.514	1.50	183.3	-1.9	47.60
288.2	5.33	0.496	1.42	214.3	1.5	47.49
291.2	4.95	0.378	1.42	260.2	-0.7	47.33
294.2	5.88	0.378	1.42	308.1	-10.3	47.16
294.2	4.86	0.313	1.50	306.8	-11.5	47.16
297.2	5.72	0.301	1.50	375.3	-11.4	46.99
300.2	6.12	0.251	1.50	479.8	12.3	46.83
303.2	7.79	0.263	1.50	580.3	17.6	46.66
306.3	6.14	0.175	1.50	685.6	7.2	46.49
309.2	5.25	0.125	1.50	819.3	14.4	46.33
4-Chloro-methylbenzene; $\Delta_1^g H_m$ (298.15 K) = (46.50 ± 0.33) kJ mol ⁻¹ $\ln(p/\text{Pa}) = \frac{262.68}{R} - \frac{63,340.57}{R \times (T, K)} - \frac{56.5}{R} \ln\left(\frac{T, K}{298.15}\right)$						
274.3	5.35	1.322	1.44	84.43	4.36	47.85
274.3	5.09	1.322	1.44	80.54	0.47	47.85
276.1	5.34	1.202	1.44	92.19	0.39	47.74
278.2	5.54	1.082	1.44	105.4	-2.0	47.63
280.2	5.74	0.961	1.44	121.8	-2.6	47.51
282.1	5.89	0.841	1.44	141.7	-0.9	47.40
285.2	6.23	0.721	1.44	173.8	-3.9	47.23
288.2	2.65	0.240	1.44	219.7	1.2	47.06
288.2	2.64	0.240	1.44	219.4	0.9	47.06
288.2	2.56	0.240	1.44	212.9	-5.6	47.06
291.3	6.42	0.481	1.44	265.3	-4.0	46.88
294.2	7.22	0.433	1.44	330.2	4.4	46.72
297.2	7.36	0.361	1.44	402.6	7.6	46.55
300.3	6.30	0.264	1.44	468.8	-10.7	46.38
303.2	4.90	0.168	1.44	571.6	-1.0	46.21
306.3	4.70	0.132	1.44	696.7	7.5	46.04
309.2	5.10	0.120	1.44	830.7	14.4	45.87

Table 3 (Continued)

T^a (K)	m^b (mg)	$V_{(N_2)}^c$ (dm ³)	Gas-flow (dm ³ h ⁻¹)	p^d (Pa)	$(p_{\text{exp}} - p_{\text{calc}})^e$ (Pa)	$\Delta_1^g H_m$ (kJ mol ⁻¹)
1-Chloro-2,6-dimethylbenzene; $\Delta_1^g H_m$ (298.15 K) = (49.78 ± 0.33) kJ mol ⁻¹ $\ln(p/\text{Pa}) = \frac{273.09}{R} - \frac{69.368.07}{R \times (T, K)} - \frac{65.7}{R} \ln\left(\frac{T, K}{298.15}\right)$						
274.5	2.65	1.931	1.93	22.46	0.25	51.34
276.2	2.23	1.451	1.28	25.01	-0.49	51.23
279.2	3.27	1.609	1.93	32.59	0.19	51.03
282.2	2.56	0.960	1.28	42.07	1.16	50.83
284.1	2.26	0.747	1.28	47.51	0.23	50.71
287.1	3.04	0.805	1.93	59.44	0.29	50.51
287.2	9.20	2.503	3.49	57.90	-1.69	50.50
290.1	5.80	1.271	2.01	71.58	-2.01	50.31
293.3	6.33	1.054	2.01	93.85	1.48	50.10
296.3	3.65	0.502	2.01	113.2	-0.5	49.90
298.2	2.81	0.342	1.28	127.5	-1.8	49.78
298.3	2.90	0.342	1.28	131.6	1.4	49.77
298.3	2.86	0.342	1.28	130.1	-0.1	49.77
300.4	3.77	0.386	1.93	151.4	1.6	49.64
305.4	3.02	0.225	1.93	207.9	0.7	49.31
1,3-Dichloro-2-methylbenzene; $\Delta_1^g H_m$ (298.15 K) = (51.60 ± 0.29) kJ mol ⁻¹ $\ln(p/\text{Pa}) = \frac{282.47}{R} - \frac{70.860.49}{R \times (T, K)} - \frac{64.6}{R} \ln\left(\frac{T, K}{298.15}\right)$						
274.2	5.19	2.486	2.98	34.03	-0.35	53.15
276.2	5.41	2.138	2.98	40.83	0.13	53.02
278.2	5.96	2.014	2.98	47.45	-0.60	52.89
280.2	6.34	1.740	2.98	57.98	1.43	52.76
282.2	6.69	1.591	2.98	66.64	0.25	52.63
284.2	6.16	1.243	2.98	78.24	0.51	52.50
288.2	8.70	1.293	2.98	105.6	-0.2	52.25
291.2	8.43	0.994	2.98	132.4	0.1	52.05
293.2	9.48	0.994	2.98	148.8	-4.4	51.92
296.2	9.01	0.746	2.98	188.1	-1.9	51.73
298.2	10.73	0.746	2.98	223.7	4.9	51.60
301.3	8.70	0.497	2.98	271.5	0.7	51.40
305.3	5.68	0.249	2.98	353.9	-0.3	51.14

^a Saturation temperature ($u(T) = 0.1$ K).

^b Mass of transferred sample m condensed at $T = 243$ K.

^c Volume of nitrogen ($u(V) = 0.005$ dm³) used to transfer m ($u(m) = 0.0001$ g) of the sample.

^d Vapor pressure at temperature T , calculated from the m and the residual vapor pressure at $T = 243$ K.

^e The combined standard uncertainty of vapor pressures measurements estimated to be within $u(p)/p = (2$ to $3)\%$, taking into account uncertainties of all variables involved in Eq. (1).

reasonable to work out the quantitative relationship. In our previous studies we have traced that the vaporization enthalpy $\Delta_1^g H_m$ (298.15 K) appears to be a linear function of the Kovat's indices in homologous series of alkylbenzenes [53]. However, fluoro- and chloro-benzenes derivatives studied in this work (see Table 1) do not belong to the homologous series. In order to reveal any quantitative structure–property relations for this series of compounds we collected Kovat's indices for species listed in Table 1 together with auxiliary indices for some parent poly-methyl substituted benzenes (see Table S3, ESI). We consider how the vaporization enthalpy correlates with the Kovat's indices [56] within methyl substituted benzenes, fluorobenzenes, and chlorobenzenes. It has turned out that the data for $\Delta_1^g H_m$ (298.15 K) also fit very well in the linear correlation. The following empirical equations for the enthalpy of vaporization have been obtained:

$$\Delta_1^g H_m(298.15 \text{ K}) / (\text{kJ mol}^{-1}) = 8.74 + 0.0388 \times J_x$$

with $(R^2 = 0.990)$ for E-101 (4)

where J_x is the Kovat's index of a substituted benzene and R^2 is the correlation coefficient. On the one hand, this relationship can be used as evidence of internal consistency of our experimental results for vaporization enthalpies. On another hand, this relationship can be used to assess enthalpies of vaporization of the parent substituted benzenes provided that their Kovat's indices are known.

3.2.2. Correlation of vaporization enthalpies $\Delta_1^g H_m$ (298.15 K) of halobenzenes with enthalpies of solution $\Delta_{\text{sol}}^g H_m$

Correlation of vaporization enthalpies with halobenzenes solution enthalpies in the stationary phase of the GC-column should be considered as a complementary method to the method based on Kovat's indices. Retention time t_r of a solute in the stationary phase is an indicator of intensity of mutual interactions. It was well established [51,53] that a plot of $\ln(1/t_r)$ vs. $1/(T/K)$, where t_r is the retention time corrected for the dead volume, results in the straight line, whose slope when multiplied by the gas constant affords $\Delta_{\text{sol}}^g H_m$ (the solution enthalpy of a solute in the stationary phase of the GC-column). It was found [57] that, in cases where compounds are properly selected with regard to the analogy of their molecular structures, plotting $\Delta_{\text{sol}}^g H_m$ versus the known standard molar vaporization enthalpy $\Delta_1^g H_m$ (298.15 K), also afford a linear relationship. This relationship can subsequently be used to evaluate the unknown vaporization enthalpy of any structurally related species provided that the unknown species is analysed at the same conditions as the standards.

There was not a lack of GC studies of halogen substituted benzenes in the literature due to awareness of their environmental impact. For our purpose we selected a reference [58] which reported an extended list of solution enthalpies of substituted benzenes in the stationary phase Apiezon L. The experimental results for the species related to the current work and their values of $\Delta_{\text{sol}}^g H_m$ are listed in Table S4 (ESI). We have observed that the correlation of vaporization enthalpies $\Delta_1^g H_m$ (298.15 K) with the solution enthalpies of substituted benzenes in Apiezon L fit very

well in the linear correlation:

$$\Delta_1^g H_m(298.15 \text{ K})/\text{kJ mol}^{-1} = 5.91 + 4.39 \times \Delta_{\text{sol}}^g H_m$$

with $(R^2 = 0.988)$ (5)

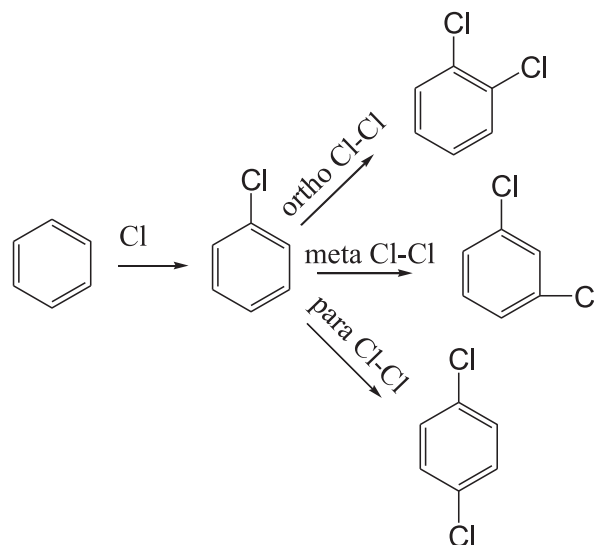
This correlation can serve as evidence of internal consistency of experimental results for vaporization enthalpies. Moreover, this relationship can be used to assess enthalpies of vaporization of some dichloro-substituted benzenes with the known solution enthalpies (see Table S4) as follows in Section 3.3.

3.3. Validation of $\Delta_1^g H_m(298.15 \text{ K})$ of chloro-dimethylbenzenes and dichloro-methylbenzenes

Having in mind the ambiguous quality of the available data for chloro-dimethylbenzenes and dichloro-methylbenzenes taken from compilations [2,3] it has been reasonable to apply the correlations according to Eqs. (4) and (5) to estimate enthalpies of vaporization of the questionable species. Comparison between two estimates with the vaporization enthalpy derived from the uncertain smoothed p - T data [2,3] should help the evaluation. Following this way we have calculated enthalpies of vaporization for a collection of substituted benzenes by using Eq. (4) (see Table 4, column 3) and Eq. (5) (see Table 4, column 5). The uncertainty of $\Delta_1^g H_m(298.15 \text{ K})$ obtained from both equations were assessed to be of $\pm 0.5 \text{ kJ mol}^{-1}$ (standard deviation). Differences between experimental values (Table 4, column 2) and the estimated values are given in columns 4 and 6 of Table 4. There are two conclusions from data comparison presented in Table 3. The first one is that estimates according to both Eqs. (4) and (5) provide reasonable values of vaporization enthalpies within $\pm 0.5 \text{ kJ mol}^{-1}$ for most compounds. The second conclusion is that two totally different GC correlations methods provide very similar vaporization enthalpies, proving consistency of the result collected and evaluated in Table 1. Due to this consistency, the experimental data available for 1,2-dichloro-4-methylbenzene, 2,4-dichloro-1-methylbenzene, and 1,4-dichloro-2,5-dimethylbenzene from compilations [3] should be excluded from thermochemical calculations and considered for revision of their primary experimental data.

3.4. Estimation of $\Delta_1^g H_m(298.15 \text{ K})$ of halogenobenzenes by group contribution method

In our previous work [6] we already reported the incremental approach to the chlorine substituted benzenes and phenols. New collection of the evaluated vaporization enthalpies listed in Tables 1 and 3 has prompted to extend the group-additivity procedure for estimation of $\Delta_1^g H_m(298.15 \text{ K})$ for more broad range of structures of substituted benzenes. In short, the difference between vaporization enthalpies of chlorobenzene and benzene provides the increment $\Delta H(\text{H} \rightarrow \text{Cl})$ for substitution of H atom on the benzene ring by Cl one. Introduction of the second chlorine atom into the benzene ring produces few additional increments (*ortho* Cl–Cl), (*para* Cl–Cl), and (*meta* Cl–Cl), taking into account the mutual interactions of substituents on the benzene ring. For example, the double Cl-substitution of H atoms of the benzene implies the following sequence of increments required for interpretation of vaporization enthalpy of poly-chloro-substituted benzenes [6]:



The following general formula for calculation of vaporization enthalpy of any polychlorobenzene (ClB) at 298.15 K can be suggested:

$$\Delta_1^g H_m(\text{ClB}) = \Delta_1^g H_m(\text{B}) + n_a \times \Delta H(\text{H} \rightarrow \text{Cl}) + n_b \times (\textit{ortho} \text{ Cl} - \text{Cl}) + n_c \times (\textit{para} \text{ Cl} - \text{Cl}) + n_d \times (\textit{meta} \text{ Cl} - \text{Cl})$$
(6)

where $\Delta_1^g H_m(\text{B})$ is vaporization enthalpy of benzene; $\Delta H(\text{H} \rightarrow \text{Cl})$ is an increment of H \rightarrow Cl substitutions on the benzene ring. The mutual interactions of the Cl atoms were taken into account through the three types of corrections in *ortho*-, *para*-, and *meta*-position on the benzene ring. n_a , n_b , n_c , n_d —are the quantities of the corresponding increments and correction. Similar approach is valid [59,60] for any kind of poly-substitution of the benzene ring (e.g. $\Delta H(\text{H} \rightarrow \text{Hal})$ for Hal=F and Cl in this work). Such a simple substitution pattern could be also applied to the toluene, xylenes, or poly-methyl benzenes using the increment $\Delta H(\text{H} \rightarrow \text{CH}_3)$ for *methyl* substituent and the appropriately modified Eq. (6) with the pairwise interactions parameters (*ortho* CH_3 – CH_3), (*para* CH_3 – CH_3), and (*meta* CH_3 – CH_3).

We used the experimental enthalpy $\Delta_1^g H_m(298.15 \text{ K})$ of benzene ($33.92 \pm 0.06 \text{ kJ mol}^{-1}$, [61], toluene ($38.06 \pm 0.04 \text{ kJ mol}^{-1}$ [61], 1,2-dimethylbenzene ($43.45 \pm 0.10 \text{ kJ mol}^{-1}$ [11], 1,3-dimethylbenzene ($42.68 \pm 0.10 \text{ kJ mol}^{-1}$ [11], 1,4-dimethylbenzene ($42.42 \pm 0.10 \text{ kJ mol}^{-1}$ [11], available from the literature together with vaporization enthalpies of fluorobenzenes and chlorobenzenes evaluated in Table 1 in order to derive increments $\Delta H(\text{H} \rightarrow \text{F})$, $\Delta H(\text{H} \rightarrow \text{Cl})$, and parameters for mutual interactions of substituents on the benzene ring (see Table 5).

Collection of parameters listed in Table 5, column 1 represents a fully detailed scheme for estimation vaporization enthalpies. For the sake of simplicity we decided to reduce as far as possible the number of parameters required for reliable prediction vaporization enthalpies of halobenzenes. Following this way we calculated the matrix of parameters listed in Table 4 with different degree of detailization. It has turned out that the mutual interactions of the *methyl* with the F or Cl-substituent can be neglected. From the (CH_3 – CH_3) interactions on the benzene ring only the *ortho*-substitution possessed a significant contribution of 1.2 kJ mol^{-1} . For the all three (Cl–Cl) interactions a common weak stabilization parameter of -1.5 kJ mol^{-1} was sufficient to reproduce the experimental data.

Comparison of the experimental and estimated vaporization enthalpies have revealed that the average deviation of

Table 4
Comparison of experimental vaporization enthalpies, $\Delta_1^{\text{g}}H_m$ (298.15 K), and those estimated using the correlation GC and group additivity (all values are in kJ mol⁻¹).

Compound	$\Delta_1^{\text{g}}H_m$ exp	$\Delta_1^{\text{g}}H_m$ Eq.(4)	Exp-calc	$\Delta_1^{\text{g}}H_m$ Eq.(5)	Exp-calc	$\Delta_1^{\text{g}}H_m$ Eq. (6)	Exp-calc
1	2	3	4	5	6	7	8
Benzene, 1,4-dichloro-	47.60 [6]	47.9	-0.3	47.2	0.4	48.2	-0.6
Benzene, 1,2-dichloro-	48.82 [6]	48.8	0.0	47.9	0.9	48.2	0.6
Benzene, 1,3-dichloro-	47.68 [6]	47.7	0.0	47.2	0.5	48.2	-0.5
Benzene, 1-chloro-4-methyl-	46.42	45.9	0.5	45.9	0.5	46.0	0.4
Benzene, 1-chloro-2-methyl-	46.14	45.7	0.5	45.9	0.2	46.0	0.1
Benzene, 1-chloro-3-methyl-	46.84	46.0	0.9	45.9	0.9	46.0	0.8
Benzene, 2-chloro-1,4-dimethyl-		49.6		49.2		50.2	
Benzene, 3,4-dichloro-1-methyl-	(56.5) ^a	52.4				52.4	
Benzene, 1,4-dichloro-2-methyl-		52.0		51.8		52.4	
Benzene, 1,3-dichloro-2-methyl-	51.60	52.0	-0.4			52.4	-0.8
Benzene, 2,4-dichloro-1-methyl-	(54.9) ^a	51.9		51.8		52.4	
Benzene, 1,4-dichloro-2,5-dimethyl-	(62.3) ^a	56.0				56.6	
Benzene, 2-chloro-1,3,5-trimethyl-		53.7				54.4	
Benzene, 4-chloro-1,2-dimethyl-		50.8				51.4	
Benzene, 1-chloro-2,4-dimethyl-		49.8		51.8		50.2	
Benzene, 1-chloro-2,3-dimethyl-		50.7				51.4	
Benzene, 2-chloro-1,3-dimethyl-	49.78	49.7	0.1			50.2	-0.4
Benzene, 3-chloro-1,2,4-trimethyl		54.6				55.6	
Benzene, 5-chloro-1,2,4-trimethyl		54.7				55.6	
Benzene, 5-chloro-1,3-dimethyl-		49.7				50.2	
Benzene, 1,3-dichloro-4,6-dimethyl		56.0				56.6	
Benzene, 1,2-dichloro-4,5-dimethyl		58.0				57.8	
Benzene, 5-chloro-1,2,3-trimethyl		55.8				56.8	
Benzene, 3-chloro-1,2-dimethyl		50.4				51.4	
Benzene, 2,3-dichloro-1,4-dimethyl				56.6		56.6	

^a Values seems to be in error.

Table 5
Parameters for the calculation of enthalpies of vaporization $\Delta_1^{\text{g}}H_m$ (298.15 K) of fluoro- and chloro-methylbenzenes.

Group contribution	Value (kJ mol ⁻¹)
Benzene	33.9
$\Delta H(H \rightarrow F)$	0.8
$\Delta H(H \rightarrow Cl)$	7.9
$\Delta H(H \rightarrow CH_3)$	4.2
<i>ortho</i> Cl–Cl	-1.5
<i>meta</i> Cl–Cl	-1.5
<i>para</i> Cl–Cl	-1.5
F–CH ₃	0.0
Cl–CH ₃	0.0
<i>ortho</i> CH ₃ –CH ₃	1.2
<i>meta</i> CH ₃ –CH ₃	0.0
<i>para</i> CH ₃ –CH ₃	0.0

experimental and calculated vaporization enthalpies on the level of 0.5 kJ mol⁻¹ quite comparable with the experimental uncertainties of the most entries in Table 1. Following, the enthalpies of vaporization of the mono- and di-halogen substituted benzenes can be predicted with acceptable accuracy using the reduced Eq. (6) with only basic increments $\Delta H(H \rightarrow \text{Hal})$ and $\Delta H(H \rightarrow \text{CH}_3)$ and with two additional increments responsible for the mutual (Cl–Cl) and *ortho* Cl–Cl interactions. It is also worse to mention, that even the consequent 1,2,3-substitution of the benzene ring with methyl or chlorine substituent for species listed in Table 1 does not require any increment specific for steric crowding of the benzene ring.

4. Conclusion

In this paper we carefully collected experimental vapor pressure and vaporization enthalpy data for fluoro- and chloro-substituted methylbenzenes available in the literature. In addition we measured vapor pressures and derived vaporization enthalpies for the series of seven halogen-substituted benzenes. We used the correlation GC method to establish consistency of the experimental data. The simple group-contribution procedure was developed for calculation enthalpies of vaporization of mono- and di-halogen

substituted benzenes which also proved the internal consistency of our experimental data. Parameters of this procedure should be transferable for prediction of vaporization enthalpies of halogenated polyaromatic compounds, dibenzodioxins or dibenzofurans.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:10.1016/j.fluid.2014.07.029.

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