Heat Capacities and Densities of Some Liquid Chloro-, Bromo-, and Bromochloro-Substituted Benzenes

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The heat capacities at constant pressure and densities of chlorobenzene (ClBz), bromobenzene (BrBz), 1,2-dichlorobenzene (1,2-DClBz), 1,3-dichlorobenzene (1,3-DClBz), 1,2-dibromobenzene (1,2-DBrBz), 1,3-dibromobenzene (1,3-DBrBz), 2-bromochlorobenzene (1,2-BrClBz), and 3-bromochlorobenzene (1,3-BrClBz) were measured within the temperature range from (283.15 to 353.15) K. The heat capacities of four other compounds [1,4-dichlorobenzene (1,4-DClBz), 1,2,3-trichlorobenzene (1,2,3-TClBz), 1,2,4-trichlorobenzene (1,2,4-TClBz), and 1,2,3,4-tetrachlorobenzene (1,2,3,4-TClBz)] were also measured between their melting point and 353.15 K. All measurements were performed by means of DSCIII (Setaram) differential scanning calorimeter. Assuming that the molar heat capacity shows an additive character, a simple equation was proposed that allows one to predict C_p values of liquid chloro and bromo derivatives of benzene as a function of temperature with an accuracy below 1 %. Densities of some of the investigated compounds were measured with the use of a DMA 5000 automatic densitometer.

Introduction

Heat capacity is one of few directly determined thermodynamic properties. In designing industrial processes as well as performing purely thermodynamic calculations, it is indispensable to know this value and its dependence on temperature. Unfortunately, the databases of physical and chemical properties still show a lack of this fundamental value, even for compounds that are often used and commercially available. Among other things, this concerns also halogeno-substituted hydrocarbons, whose heat capacities and their dependences on temperature have also been investigated by us earlier.[1−3]

Beside the basic objective to obtain reliable and precise data of C_p as a function of temperature, the obtained experimental data are used to develop models describing the effect of compound structure on the value of C_p. As follows from our papers,[2,3] in the case of mono- and dihalogeno-substituted alkanes it is possible to use a simple additivity model to describe the dependence of C_p on the of alkyl chain length and temperature. The calculated C_p contributions of groups that form these compounds can be useful to predict the C_p values of compounds, whose data are missing in the literature.

The present work is a continuation of these studies, attempting to divide the value of C_p into group contributions for several halogen derivatives of benzene. The database to carry out these calculations consists of directly measured C_p values for 12 chloro- and/or bromo-substituted benzenes with a number of substitutes from one to four within the temperature range from (283 to 353) K.

Experimental Section

Chemicals. Chlorobenzene (Aldrich, ≥99.5 %), bromobenzene (Aldrich, ≥99 %), 1,3-bromochlorobenzene (Aldrich, 99 %), 1,2-dichlorobenzene (Aldrich, 99 %), 1,4-dichlorobenzene (Aldrich, ≥99 %), 1,2,3-trichlorobenzene (Aldrich, 99 %), and 1,2,4-trichlorobenzene (Aldrich, ≥99 %) were used without further purification. The 1,2-bromochlorobenzene (Aldrich, 99 %), 1,3-dichlorobenzene (Aldrich, 98 %), 1,2-dibromobenzene (Aldrich, 98 %), 1,3-dibromobenzene (Aldrich, 97 %), and 1,2,4,5-tetrachlorobenzene (Aldrich, 98 %) were purified by fractional distillation under reduced pressure. The final purity of the compounds used for experiments was determined by the method of thermal analysis using s DSC 111 (Setaram) calorimeter to be ≥ 99 mol %. Prior to the measurements, all chemicals were dried with activated molecular sieves (type 4Å from Lancaster) and degassed in an ultrasonic stream.

Table 1. Comparison of the Experimental and Literature Data of Heat Capacity (C_p/J·mol^{-1}·K^{-1}) and Density (d/g·cm^{-3}) (T = 298.15 K)

	C_p/J·mol^{-1}·K^{-1}		d/g·cm^{-3}	
compound	this work	literature	this work	literature
chlorobenzene	150.96	150.70[4]	1.10114	1.10100[9]
bromobenzene	154.77	154.29[5]	1.48845	1.48818[9]
1,2-dichlorobenzene	170.68	170.61[6], 171.16[7]	1.30061	1.30033[10]
1,3-dichlorobenzene	170.18	169.80[6], 170.01[7]	1.28279	1.28280[5]
1,2,4-trichlorobenzene	195.07	194.25[6], 194.46[7] 194.55[8]	1.44867	1.44815[8]

Apparatus and Procedure. The differential scanning calorimetry (DSC), applied in this study, is one of the modern analytical techniques often used since a quantitative information can be obtained over a wide range of temperatures from small (1 mL) samples. The saturated specific heat capacities were measured by means of a high sensitivity DSC Micro DSC III (Setaram) based on the Tian-Calvet's principle. The "continuous with reference" method (*n*-heptane as a reference) was applied. Details of the applied procedure and the calorimeter calibration have been described previously.[2] Thanks to some changes[2] made in relation to the standard measurement technique, the uncertainty of the C_p values obtained in this work did not exceed ± 0.15 %. The samples were weighed with a Sartorius RC 210D balance with an accuracy of $2\cdot10^{-5}$g and were filled in the drybox.

The density measurements were performed using an Anton Paar density analyzer DMA 5000 with an accuracy of $5\cdot10^{-6}$ g·cm^{-3}. The comparison of obtained values of C_p and density

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Table 2. Molar Heat Capacities (C_p/J·mol^{-1}·K^{-1}) for Some Chloro-Substituted Benzene Derivatives in the Temperature Range from T = 283.15 K to T = 353.15 K

T	C_p/J·mol^{-1}·K^{-1}						
K	ClBz	1,2-DClBz	1,3-DClBz	1,4-DClBz	1,2,3-TClBz	1,2,4-TClBz	1,2,3,4-TClBz
283.15	147.73	167.68	167.15				
285.15	148.14	168.06	167.54				
287.15	148.56	168.44	167.93				
289.15	148.99	168.83	168.32				
291.15	149.41	169.23	168.72				
293.15	149.85	169.64	169.13			194.25	
295.15	150.29	170.05	169.55			194.57	
297.15	150.73	170.47	169.97			194.90	
299.15	151.18	170.89	170.39			195.23	
301.15	151.64	171.32	170.82			195.57	
303.15	152.10	171.76	171.25			195.92	
305.15	152.56	172.20	171.69			196.27	
307.15	153.03	172.64	172.14			196.63	
309.15	153.50	173.09	172.58			196.99	
311.15	153.97	173.54	173.04			197.35	
313.15	154.45	174.00	173.49			197.72	
315.15	154.93	174.46	173.95			198.09	
317.15	155.41	174.92	174.41			198.47	
319.15	155.90	175.38	174.88			198.85	
321.15	156.39	175.85	175.35			199.23	
323.15	156.88	176.32	175.83			199.61	
325.15	157.37	176.79	176.30			200.00	
327.15	157.86	177.26	176.78	177.09	201.44	200.38	225.17
329.15	158.36	177.73	177.26	177.53	201.80	200.77	225.49
331.15	158.86	178.20	177.75	177.98	202.16	201.16	225.82
333.15	159.35	178.67	178.24	178.43	202.52	201.55	226.14
335.15	159.85	179.14	178.73	178.89	202.88	201.93	226.47
337.15	160.35	179.61	179.22	179.35	203.25	202.32	226.80
339.15	160.85	180.07	179.71	179.81	203.62	202.71	227.13
341.15	161.35	180.54	180.20	180.28	204.00	203.09	227.46
343.15	161.85	181.00	180.70	180.76	204.38	203.47	227.80
345.15	162.35	181.47	181.20	181.24	204.75	203.85	228.13
347.15	162.85	181.92	181.70	181.73	205.14	204.23	228.47
349.15	163.34	182.38	182.20	182.22	205.52	204.61	228.81
351.15	163.84	182.83	182.70	182.71	205.91	204.98	229.16
353.15	164.34	183.28	183.20	183.21	206.30	205.35	229.50

together with the data available in the literature for 298.15 K are listed in Table 1. As is seen, there is a good agreement of both C_p and densities at 298.15 K, and in the case of C_p, the differences usually do not exceed 0.25 %. For the remaining compounds under investigation, there are no data determined at 298.15 K with satisfactory precision (densities) or no data at all in the literature.

Results

The measurements of the saturated heat capacity of the examined halogen derivatives of benzene were generally performed within the temperature range from (283 to 353) K. For the four compounds (1,4-dichlorobenzene, 1,2,3-trichlorobenzene, 1,2,4-trichlorobenzene, and 1,2,4,5-tetrachlorobenzene) that are solid at 283 K, the measurements were carried out in the range between its melting points and 353 K.

The applied DSC continuous method gives a set of ca. 3500 data points over the examined temperature range. For clarity, only the C_p values obtained every 2.0 K are presented in Tables 2 and 3.

Directly determined molar heat capacities as a function of temperature were fitted to the following equation:

$$C_p/\mathrm{J{\cdot}mol^{-1}{\cdot}K^{-1}} = \sum_{i=0}^{2} A_i (T/\mathrm{K} - 293.15)^i \qquad (1)$$

where A_i are constants determined by the least-square method and are collected in Table 4.

Astonishingly few data of density, especially as a function of temperature, for the investigated group of compounds are available in the literature. This has prompted us to present the values determined by us of density for nine benzene derivative that are liquid within the temperature range from T = (288.15 to 323.15) K (Table 5).

Group Additivity Analysis of Heat Capacity. The group additivity method assumes that various groups of the molecule contribute definitive values to the total molar heat capacity. The calculated C_p values of particular groups and their dependencies on temperature allow us to foresee the C_p values of relatively simple chemical compounds. However, the accuracy of these forecasts depends on many factors. The most important of them include the precision of initial C_p data used as the basis for analysis, available range of temperature, and number of compounds involved in the analysis. The precision of estimation usually goes down with the increase in the number of functional groups in the given compound and their reciprocal effects, for example, as a result of the proximity effect.

In the case of the investigated herein chloro- and bromo derivatives of benzene, the model of simple additivity suggest a division restricted only to two or three functional groups such as CH, CBr, and CCl. According to preliminary calculations, the use of such a simple model brings about a situation where the deviation of estimated C_p values from experimental data increases with the number of halogen substituents in the ring. In the case of multi-substituted halogenobenzenes, one can observe some nonlinear increase in C_p values with the number of substituents, connected with "accumulation" of halogen in

Table 3. Molar Heat Capacities (C_p/J·mol^{-1}·K^{-1}) for Some Bromo- and Bromochloro-Substituted Benzene Derivatives in the Temperature Range from T = 283.15 K to T = 353.15 K

T	C_p/J·mol^{-1}·K^{-1}					T	C_p/J·mol^{-1}·K^{-1}				
K	BrBz	1,2-DBrBz	1,3-DBrBz	1,2-BrClBz	1,3-BrClBz	K	BrBz	1,2-DBrBz	1,3-DBrBz	1,2-BrClBz	1,3-BrClBz
283.15	151.63	177.44	176.01	172.25	171.14	319.15	159.20	183.97	182.85	179.31	178.44
285.15	151.99	177.83	176.40	172.59	171.49	321.15	159.66	184.38	183.28	179.74	178.89
287.15	152.37	178.12	176.71	172.94	171.84	323.15	160.13	184.79	183.70	180.17	179.33
289.15	152.75	178.43	177.04	173.29	172.21	325.15	160.60	185.19	184.13	180.60	179.78
291.15	153.14	178.75	177.38	173.65	172.59	327.15	161.06	185.60	184.55	181.03	180.23
293.15	153.54	179.08	177.72	174.02	172.97	329.15	161.53	186.01	184.98	181.47	180.68
295.15	153.94	179.42	178.08	174.39	173.36	331.15	162.00	186.42	185.40	181.90	181.13
297.15	154.35	179.76	178.44	174.78	173.75	333.15	162.48	186.82	185.83	182.33	181.58
299.15	154.77	180.12	178.81	175.17	174.15	335.15	162.95	187.23	186.25	182.77	182.03
301.15	155.19	180.48	179.19	175.56	174.56	337.15	163.42	187.63	186.67	183.20	182.47
303.15	155.62	180.85	179.58	175.96	174.98	339.15	163.89	188.03	187.08	183.62	182.92
305.15	156.05	181.22	179.97	176.36	175.40	341.15	164.36	188.42	187.49	184.05	183.36
307.15	156.49	181.60	180.37	176.77	175.82	343.15	164.83	188.82	187.90	184.47	183.80
309.15	156.93	181.99	180.78	177.19	176.25	345.15	165.30	189.20	188.30	184.89	184.24
311.15	157.38	182.38	181.19	177.61	176.68	347.15	165.76	189.58	188.70	185.31	184.67
313.15	157.83	182.77	181.60	178.03	177.12	349.15	166.23	189.96	189.09	185.72	185.10
315.15	158.28	183.17	182.01	178.45	177.56	351.15	166.69	190.33	189.47	186.13	185.52
317.15	158.74	183.57	182.43	178.88	178.00	353.15	167.15	190.69	189.85	186.53	185.94

Table 4. Coefficients of the Polynomial (1) and Mean Deviation from the Regression Line

		coefficients of eq 1			
	temp. range	A	A_1·10^2	A_2·10^4	δC_p
compound	K	J·mol^{-1}·K^{-1}	J·mol^{-1}·K^{-2}	J·mol^{-1}·K^{-3}	J·mol^{-1}·K^{-1}
ClBz	283−353	149.895 ± 0.001	22.40 ± 0.01	2.86 ± 0.02	0.04
1,2-DClBz	283−353	169.659 ± 0.002	21.46 ± 0.02	2.25 ± 0.03	0.10
1,3-DClBz	283−353	169.143 ± 0.001	20.99 ± 0.01	4.17 ± 0.02	0.06
1,4-DClBz	327−353	170.340 ± 0.006	17.76 ± 0.03	6.15 ± 0.03	0.12
1,2,3-TClBz	327−353	196.034 ± 0.026	14.41 ± 0.10	4.25 ± 0.10	0.04
1,2,4-TClBz	293−353	194.275 ± 0.002	16.82 ± 0.02	2.99 ± 0.03	0.10
1,2,3,4-TClBz	327−353	220.286 ± 0.008	12.98 ± 0.04	3.87 ± 0.04	0.12
BrBz	283−353	153.559 ± 0.002	20.87 ± 0.01	3.28 ± 0.03	0.08
1,2-DBrBz	283−353	179.112 ± 0.002	18.12 ± 0.02	2.31 ± 0.03	0.12
1,3-DBrBz	283−353	177.753 ± 0.002	19.06 ± 0.02	2.23 ± 0.03	0.11
1,2-BrClBz	283−353	174.013 ± 0.003	19.64 ± 0.02	2.13 ± 0.04	0.10
1,3-BrClBz	283−353	173.038 ± 0.003	20.51 ± 0.02	1.96 ± 0.04	0.10

Table 5. Densities of Some Investigated Halogen-Substituted Benzenes as a Function of Temperature

	d/g·cm^{-3}					
compound	288.15 K	298.15 K	308.15 K	318.15 K	328.15 K	338.15 K
ClBz	1.11190	1.10114	1.09034	1.07948	1.06857	1.05758
1,2-DClBz	1.31176	1.30061	1.28945	1.27829	1.26709	1.25587
1,3-DClBz	1.29408	1.28279	1.27149	1.26017	1.24882	1.23742
1,2,4-TClBz	1.46065	1.44867	1.43673	1.42480	1.41289	1.40098
BrBz	1.50195	1.48845	1.47494	1.46139	1.44780	1.43415
1,2-DBrBz	1.98792	1.97275	1.95762	1.94251	1.92742	1.91234
1,3-DBrBz	1.96414	1.94887	1.93361	1.91830	1.90313	1.88788
1,2-BrClBz	1.65967	1.64632	1.63301	1.61969	1.60636	1.59303
1,3-BrClBz	1.63844	1.62497	1.61151	1.59805	1.58456	1.57105

the same aromatic ring. Therefore, the C_p value of any chloro-, bromo-, and bromochlorobenzenes with the general formula $C_6H_{(6-x-y)}Cl_xBr_y$ has been described by us by an empirical relationship that takes into account this phenomenon as the last term of the expression:

$$C_p = n_{CH}C_p(CH) + n_{CBr}C_p^*(CBr) + n_{CCl}C_p^*(CCl) + d\cdot(n_{CBr} + n_{CCl})^2 \quad (2)$$

where n_{CH}, n_{CBr}, and n_{CCl} are the number of CH, CBr, and CCl groups in the ring, respectively; C_p(CH) defines the contribution of CH group to the molar heat capacity of the compound; C_p^*(CCl), C_p^*(CBr), and d are the adjustable parameters having no direct physical meaning.

The last term of eq 2 takes into account the increase in molar C_p of the compound caused by the "accumulation" of halogen substituents in the ring. This effect is independent of the type of halogen substituent. Thus, the contribution of CBr and CCl groups to the molar heat capacity of the whole compound is not constant, but it increases with the total number of halogen substituents.

The contributions of CBr and CCl groups to the heat capacity of the compound are given by the following linear equations:

$$C_p(CCl) = C_p^*(CCl) + d\cdot(n_{CBr} + n_{CCl}) \quad (3)$$

for CCl group, and analogously

$$C_p(CBr) = C_p^*(CBr) + d\cdot(n_{CBr} + n_{CCl}) \quad (4)$$

for the CBr group. In eqs 3 and 4, C_p^*(CBr) and C_p^*(CCl) have no physical sense as they define the heat capacity of the given group when $n_{CBr} + n_{CCl} = 0$ (no substituents in the ring). In compounds substituted with, for example, four substituents of

Table 6. Coefficients of Equation 5 and Their Standard Deviations

a_0/J·mol^{-1}·K^{-1}	a_1/J·mol^{-1}·K^{-2}
22.4610 ± 0.0130	0.0378 ± 0.0004
b_0	b_1
34.5763 ± 0.1175	0.0803 ± 0.0037
c_0	c_1
39.0255 ± 0.1039	0.0614 ± 0.0033
d_0	d_1
2.5737 ±0.0431	−0.0200 ±0.0014

the given type, all CCl (or CBr) groups have the same group heat capacity expressed by one of the eqs (eq 3 or 4), where ($n_{CBr} + n_{CCl}$) is equal to four. The same heat capacity is shown by the CCl (or CBr) group in all other four-substituted compounds, for example, dibromodichloro- or tribromochloro-substituted compounds (the sum $n_{Cl} + n_{Br}$ is equal also to four).

The degree of polynomials properly describing the temperature dependence of C_p is seldom higher than 3. Thus, eq 2 may be written in the following form:

$$C_p/\mathrm{J\cdot mol^{-1}\cdot K^{-1}} = n_{CH}\sum_{i=0}^{1} a_i(T/\mathrm{K} - 293.15)^i + n_{CCl}\sum_{i=0}^{1} b_i(T/\mathrm{K} - 293.15)^i + n_{CBr}\sum_{i=0}^{1} c_i(T/\mathrm{K} - 293.15)^i + (n_{CCl} + n_{CBr})^2\sum_{i=0}^{1} d_i(T/\mathrm{K} - 293.15)^i \quad (5)$$

where C_p is the molar heat capacity; T is the temperature; n_{CH}, n_{CBr}, and n_{CCl} have the same meaning as in eq 2; and a_i, b_i, c_i, and d_i are the fitting parameters listed in Table 2.

The database used to determine the parameters of eq 5 consisted of the C_p values of all 12 compounds (Tables 2 and 3) investigated by us and additionally the literature data for benzene.[11] The values of coefficients of eq 5 and their standard deviations are given in Table 6.

Equation 5 describes the C_p values for several chloro-, bromo-, and bromochloro-substituted benzenes with an average deviation from experimental data amounting to ± 0.4 %. An exception comes from 1,2,3-TClBz over 333 K and 1,2-DChBz below 288 K, where the deviation is about 0.7 %. It is essential that the calculated contribution of C_p of CH group very well describes also the temperature dependence of heat capacity of non-substituted benzene. The deviation from the literature value[11] is below 0.1 % within the range from (293 to 323) K and about 0.2 % below and above temperatures of this range.

In the literature, one can find C_p data of four liquid halogen-substituted benzenes not investigated in this work: 1,4-dibromobenzene[12] (1,4-DBrBz), 1,3,5-trichlorobenzene[6,12] (1,3,5-TChBz), 1,3,5-tribromobenzene[12] (1,3,5-TBrBz), and pentachlorobenzene[6] (PChBz). These data concern the temperature range above 353 K, which is due to the high melting points of these derivatives. Rohac et al.[6] and van Miltenburg et al.[13] have also determined C_p values of several other chloro derivatives of benzene at temperatures higher than 353 K.

The comparison of C_p values calculated from eq 5 and available experimental data within the range above 353 K (from 377 to 395 K) are listed in Table 7. As is seen, the discrepancy of estimated and experimental C_p values is at the average 0.5 %, usually being comparable with the accuracy of the experimental data cited in the literature. One should bear in mind that

Table 7. Comparison of Experimental and Calculated C_p/J·mol^{-1}·K^{-1} Values from Equation 5 of Several Halogen-Substituted Benzenes at Temperatures up to T = 395 K

	T	C_p/J·mol^{-1}·K^{-1}		deviation[a]
compound	K	eq 5	literature	%
1,2-DClBz	377	188.73	189.48[6,b]	0.40
	395	192.90	194.16[6,b]	0.65
1,3-DClBz	377	188.73	188.72[6,b]	0.00
	395	192.90	192.95[6,b]	0.03
1,4-DClBz	380	189.42	188.66[12,c]	0.40
	380	189.42	189.91[6,b]	0.26
	395	192.90	193.47[6,b]	0.29
1,4-DBrBz	380	195.04	194.61[12,c]	0.22
1,3-BrClBz	360	187.97	187.83[13,c]	0.07
	370	190.10	190.08[13,c]	0.01
1,2,3-TClBz	377	208.89	210.60[6,b]	0.81
	395	212.03	213.91[6,b]	0.88
1,2,4-TClBz	377	208.89	209.81[6,b]	0.44
	395	212.03	213.37[6,b]	0.63
1,3,5-TClBz	380	209.41	207.79[12,c]	0.78
	380	209.41	209.64[6,b]	0.11
	395	212.03	212.99[6,b]	0.45
1,3,5-TBrBz	395	219.60	220.85[12,c]	0.57
pentachlorobenzene	368	255.14	253.99[6,b]	0.45
	385	254.11	256.28[6,b]	0.85

[a] Deviation of C_p values calculated from eq 5 from experimental data $(C_p^{exp} - C_p^{calc})\cdot 100/C_p^{exp}$. [b] Experimental uncertainty 1 %. [c] Experimental uncertainty 0.2 %.

the coefficients of eq 5 were calculated mainly on the basis of experimental database for two substituted compounds (seven compounds), and they relate to the temperature range from (283 to 353) K. Thus, the estimated value of C_p (e.g., for pentachlorobenzene) constitutes extrapolation in terms of both temperature (by about 30°) and the number of substituents. As is seen from Table 7, in all the cited cases, the estimation error does not exceed 1 % despite the temperature extrapolation up to 395 K (i.e., more than 40° over the temperatures of our measurements).

The high conformity of the C_p values calculated from eq 5 with the available experimental data indicates that this equation can be successfully used to predict C_p values of liquid chloro, bromo, or bromochloro derivatives of benzene whose C_p data are missing in the literature.

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