Thermochimica Acta, 213 (1993) 1–10
Elsevier Science Publishers B.V., Amsterdam

Heat capacity at constant pressure of some halogen compounds

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(Received 20 April 1992)

Abstract

Constant-pressure heat capacity values at 298.15 K and 308.15 K of some liquid halogenated hydrocarbons of the types $X(CH_2)_nX$ and RX, where X = Cl, Br and I and R = alkyl or phenyl group, have been measured by using a precise micro drop heat-capacity calorimeter. A comparison is made between the experimental results and the values calculated from group contribution methods. Values for the heat capacity are discussed in terms of group additives. Some improved additive parameters and a group contribution method for the prediction of the heat capacity values are proposed. The new method gives more accurate predictions than earlier relationships.

INTRODUCTION

Heat capacity is a fundamental thermodynamic property of substances. Accurate values for the specific heat capacities at constant pressure C_p of pure liquids and their mixtures are often needed in process calculation or in modelling of thermodynamic properties. The heat capacities of halogen compounds are rarely found in the literature. Therefore, these values at 298.15 K and 308.15 K and 1 atm for compounds of the types $X(CH_2)_nX$ and RX, where X = Cl, Br or I and R = alkyl or phenyl groups, were determined using the drop heat-capacity calorimeter [1]. In addition, a simple method for the estimation of the heat capacity of liquids, especially for liquid halogenated hydrocarbons, was developed.

EXPERIMENTAL

Materials

Reagent-grade water produced by a Milli-Q filtration system was used in the calibration experiments. Prior to filling the ampoule in the cali-

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bration experiments, dissolved gases were removed from the water by boiling. All samples were of commercial origin (Fluka, BDH, Aldrich and Sigma). The samples were dried with Drierite and purified by fractional distillation until their purities, as estimated by gas chromatography were ≥99.9 mol.%. All prepared substances were protected from the effects of light. The iodides were stored in darkness and to prevent decomposition, a piece of silver wool was added to the storage ampoules [2, 3].

Calorimetry

The heat capacities of the substances were measured using a micro drop heat-capacity calorimeter [1]. The stainless steel ampoule was filled with approx. 0.6 cm^3 of sample. It was equilibrated in the furnace near 301.15 K (or 313.15 K) before the drop. At a pre-programmed time it was then transferred by free fall to the receiving calorimeter, which was kept near 295.15 K (or 303.15 K) and the resulting heat transfer through the thermopile's plate was measured. The calorimeter was calibrated with water using the C_p^* values of 4.1797 and 4.1782 $J\,K^{-1}\,g^{-1}$ [4] at 298.15 K and 308.15 K, respectively. The mean temperature in all cases was 298.15 ± 0.05 K and 308.15 ± 0.05 K.

Calculations

Calculations of the results were described in detail earlier [1, 5] and only a brief account will be given here. The heat quantity q transferred through the thermocouple plates is equal to the product of the recorded integral of potential V with respect to time Δt, and a calibration constant ε

$$q = \varepsilon \sum V \Delta t$$

From the measured value of $\Delta\theta$ = furnace temperature − calorimeter temperature, the heat capacity of the ampoule and its contents C_{tot} can be calculated

$$C_{tot} = q/\Delta\theta$$

The heat capacity for the sample can be calculated from the difference in experimental results carried out with the ampoule filled and empty.

RESULTS AND DISCUSSION

Results from the calorimetric measurements are summarized in Tables 1–5. Each value reported is the mean of four or more ampoule fillings and they were repeated seven to eleven times on each filling. The uncertainties

TABLE 1

Molar heat capacity values of some monohalogen compounds RX at 298.15 K

R	C_p^* (J mol^{-1} K^{-1})			CH$_2$ increment (J mol^{-1} K^{-1})		
	X = Cl	X = Br	X = I	X = Cl	X = Br	X = I
Methyl	–	–	82.0 ± 0.3			
				–	–	27.7
Ethyl	–	105.8 ± 0.2	109.7 ± 0.1			
				–	28.8	26.5
Propyl	132.2 [a]	134.6 ± 0.2	136.2 ± 0.2			
				26.7	27.6	28.3
Butyl	158.9 ± 0.2	162.2 ± 0.2	164.5 ± 0.1			
				28.8	28.8	29.1
Pentyl	187.7 ± 0.2	191.0 ± 0.2	193.6 ± 0.2			
				28.5	28.7	28.9
Hexyl	216.2 ± 0.2	219.7 ± 0.2	222.5 ± 0.3			
				29.2	28.2	29.3
Heptyl	245.4 ± 0.3	247.9 ± 0.3	251.8 ± 0.3			
				29.3	–	–
Octyl	274.7 ± 0.3	–	–			
				–	28.1	28.2
iso-Propyl	–	135.6 ± 0.2	137.3 ± 0.2			
				–	–	–
iso-Butyl	–	163.7 ± 0.2	165.5 ± 0.2			
				–	–	–
sec-Butyl	160.9 ± 0.2	–	165.3 ± 0.2			
				–	–	–
tert-Butyl	162.0 ± 0.3	165.7 ± 0.1	–			
				–	–	–
Cyclohexyl	–	182.1 ± 0.2	–			
				–	–	–
Phenyl	152.1 ± 0.2	155.2 [b]	158.4 ± 0.1			

[a] Ref. 6. [b] Refs. 7 and 8.

TABLE 2

Molar heat capacity values of some α,ω-dihalogen compounds at 298.15 K

Compound	C_p^* (J mol^{-1} K^{-1})			CH$_2$ increment (J mol^{-1} K^{-1})		
	X = Cl	X = Br	X = I	X = Cl	X = Br	X = I
XCH_2X	100.9 [a]	104.1 ± 0.2	112.8 ± 0.2			
				28.5	30.6	–
$X(CH_2)_2X$	129.4 ± 0.2 [b]	134.7 ± 0.2	–			
				27.6	29.0	–
$X(CH_2)_3X$	157.0 ± 0.2 [b]	163.7 ± 0.2	169.2 ± 0.2			
				27.0	27.5	–
$X(CH_2)_4X$	184.0 ± 0.2 [b]	191.2 ± 0.2	–			
				29.4	–	–
$X(CH_2)_5X$	213.4 ± 0.2 [b]	–	–			

[a] Ref. 6. [b] Ref. 9.

TABLE 3

Molar heat capacity values (J mol^{-1} K^{-1}) of chloroform and carbon tetrachloride at 298.15 K

Compound	Present work	Literature value
$CHCl_3$	113.2 ± 0.2	113.8 [a], 115.5 [b]
CCl_4	131.3 ± 0.2	132.6 [b], 131.8 [c], 131.4 [d]

[a] Ref. 10. [b] Ref. 8. [c] Ref. 11. [d] Ref. 6.

given in the tables are random errors expressed as twice the standard deviation of the mean. Tables 1, 2, 4 and 5 list CH_2 increments for the investigated homologous series. In Table 6, a comparison is made between the present results and those available literature values at 298.15 K. Also, in Tables 7 and 8 a comparison is made between the present results and the calculated values from the group contributions for the Missenard and Chueh–Swanson methods [14–16] at 298.15 K. In the Missenard method, the heat capacity values were calculated from the thermal conductivity, but in the Chueh–Swanson method, they started from Watson's [17] suggestion that the heat capacity be calculated from the vapour heat capacity and the heat of vaporization.

TABLE 4

Molar heat capacity values of some monohalogen compounds RX at 308.15 K

R	C_p^* (J mol^{-1} K^{-1})			CH_2 increment (J mol^{-1} K^{-1})		
	X = Cl	X = Br	X = I	X = Cl	X = Br	X = I
Methyl	–	–	–			
				–	–	–
Ethyl	–	–	–			
				–	–	–
Propyl	–	135.6 ± 0.2	137.8 ± 0.2			
				–	29.2	29.3
Butyl	161.5 ± 0.2	164.8 ± 0.2	167.1 ± 0.2			
				29.2	29.0	29.4
Pentyl	190.8 ± 0.2	193.8 ± 0.2	196.5 ± 0.2			
				29.5	29.1	29.6
Hexyl	220.3 ± 0.2	222.9 ± 0.2	226.1 ± 0.2			
				29.6	29.1	29.9
Heptyl	249.9 ± 0.3	252.0 ± 0.2	256.0 ± 0.2			
				29.5	–	–
Octyl	279.4 ± 0.3	–	–			
Phenyl	153.2 ± 0.2	156.8 ± 0.3	160.6 ± 0.2			

TABLE 5

Molar heat capacity values of some α,ω-dihalogen compounds at 308.15 K

Compound	C_p^* (J mol^{-1} K^{-1})			CH$_2$ increment (J mol^{-1} K^{-1})		
	X = Cl	X = Br	X = I	X = Cl	X = Br	X = I
XCH_2X	–	104.6 ± 0.2	113.6 ± 0.2			
				–	31.9	–
$X(CH_2)_2X$	130.1 ± 0.1	136.5 ± 0.2	–			
				28.7	29.0	–
$X(CH_2)_3X$	158.8 ± 0.2	165.5 ± 0.2	171.3 ± 0.2			
				28.7	28.3	–
$X(CH_2)_4X$	187.5 ± 0.2	193.8 ± 0.2	–			
				28.7	–	–
$X(CH_2)_5X$	216.2 ± 0.2	–	–			

The comparisons show that

(1) There is good agreement between the experimental and the literature values.

(2) There is fair agreement between the calculated and experimental values for all straight-chain monohalogen compounds.

(3) There is a considerable difference between the two sets of values for α,ω-dihalogen compounds.

(4) For the branched compounds:

iso-Propyl bromide and iodide: there is a difference between the experimental and the corresponding calculated values for both methods of calculation.

iso-Butyl bromide and *sec*-butyl chloride: the experimental values are in good agreement with those calculated by the Chueh–Swanson method but they are lower than the values calculated by Missenard's method.

TABLE 6

Comparison between the present and literature molar heat capacity values (J mol^{-1} K^{-1}) at 298.15 K

Compound	Present work	Literature value
$Cl(CH_2)_2Cl$	129.4 ± 0.2	129.3 [a]
$Br(CH_2)_2Br$	134.7 ± 0.2	134.7 [b]
$CHCl_3$	113.2 ± 0.2	113.8 [a], 115.5 [b]
CCl_4	131.3 ± 0.2	132.6 [b], 131.8 [c], 131.4 [d]
CH_3I	82.0 ± 0.3	82.9 [e]
CH_3CH_2I	109.7 ± 0.1	109.0 [f]

[a] Ref. 10. [b] Ref. 8. [c] Ref. 11. [d] Ref. 6. [e] Ref. 12. [f] Ref. 13.

TABLE 7

Comparison between experimental and calculated molar heat capacity values (J mol^{-1} K^{-1}) of monohalogen compounds RX at 298.15 K

R	X = Cl			X = Br			X = I		
	Exp.	Calc.[a]	Calc.[b]	Exp.	Calc.[a]	Calc.[b]	Exp.	Calc.[a]	Calc.[b]
Methyl	–	–	–	–	–	–	82.0	82.0	72.8
Ethyl	–	–	–	105.8	105.9	105.2	109.7	110.2	103.2
Propyl	132.2	127.9	133.2	134.6	134.1	135.6	136.2	138.5	133.6
Butyl	158.9	156.1	163.6	162.2	162.3	166.0	164.5	166.7	164.0
Pentyl	187.7	184.3	194.0	191.0	190.6	196.4	193.6	195.0	194.4
Hexyl	216.2	212.6	224.4	219.7	218.8	226.8	222.5	223.2	224.8
Heptyl	245.4	240.8	254.8	247.9	247.0	257.2	251.8	251.5	255.2
Octyl	274.7	269.0	285.6	–	–	–	–	–	–
iso-Propyl	–	–	–	135.6	144.1	132.6	137.3	148.5	130.6
iso-Butyl	–	–	–	163.7	172.3	163.0	165.5	176.8	161.0
sec-Butyl	160.9	166.1	161.0	–	–	–	165.3	176.8	161.0
tert-Butyl	162.0	163.0	153.8	165.7	169.2	155.8	–	–	–
Cyclohexyl	–	–	–	182.1	188.0	185.8	–	–	–
Phenyl	152.1	146.9	159.0	155.2[c]	153.1	160.7	158.4	157.5	159.0

[a] Ref. 14. [b] Ref. 15. [c] Refs. 7 and 8.

iso, *sec* and *tert*-Butyl iodide: the experimental values fall between both calculated values.

tert-Butyl bromide and *tert*-butyl chloride: the experimental values are in fair agreement with those calculated by Missenard, but both are higher than Chueh and Swanson's calculated values.

(5) There is good agreement between the experimental and calculated values for iodo-benzene. For chloro- and bromo-benzene, the experimental values are intermediate values.

TABLE 8

Comparison between experimental and calculated molar heat capacity values (J mol^{-1} K^{-1}) of α,ω-dihalogen compounds at 298.15 K

Compound	X = Cl			X = Br			X = I		
	Exp.	Calc.[a]	Calc.[b]	Exp.	Calc.[a]	Calc.[b]	Exp.	Calc.[a]	Calc.[b]
XCH_2X	100.9	87.6	102.4	104.1	100.2	106.4	112.8	109.0	102.4
$X(CH_2)_2X$	129.4	115.9	132.8	134.7	128.4	136.8	–	–	–
$X(CH_2)_3X$	157.0	144.2	163.2	163.7	156.7	167.2	169.2	165.5	163.2
$X(CH_2)_4X$	184.0	172.4	193.6	191.2	184.9	197.6	–	–	–
$X(CH_2)_5X$	213.4	200.4	224.0	–	–	–	–	–	–

[a] Ref. 14. [b] Ref. 15.

(6) For cyclohexyl bromide, there is good agreement between experimental and calculated values.

Some correlations between the structure and heat capacity

CH_2 increments

Tables 1 and 2 list CH_2 increments at 298.15 K for straight-chain halogenated hydrocarbons. It is evident that there is fair constancy within each group. For both mono- and dihalogen compounds there is average CH_2-increment values of 28.42 J K^{-1} mol^{-1} at 298.15 K, which is in good agreement with that reported earlier by Missenard (28.2 J K^{-1} mol^{-1}). It is lower than the Chueh–Swanson value (30.4 J K^{-1} mol^{-1}).

Halogen group value

Figure 1 shows C_p^* values of α,ω-dibromoalkanes at 298.15 K plotted versus the number of methylene groups N_{CH_2}. It can be seen that there is a constant increase in the value of C_p^* with the number of methylene groups. Extrapolation of the line to $N_{CH_2} = 0$ yields an intercept value of 75.85 ± 1.34 J K^{-1} mol^{-1} (1.34 represents the standard deviation of the intercept) corresponding to the C_p^* value of Br_2, which is in good agreement with the literature value [7] (75.69 J K^{-1} mol^{-1}). This leads to the C_p^* group parameter value for the bromine atom, $\phi(Br) =$ 37.93 J K^{-1} mol^{-1}. This value is the same as that reported earlier by Chueh and Swanson (38 J K^{-1} mol^{-1}). By looking at the different series,

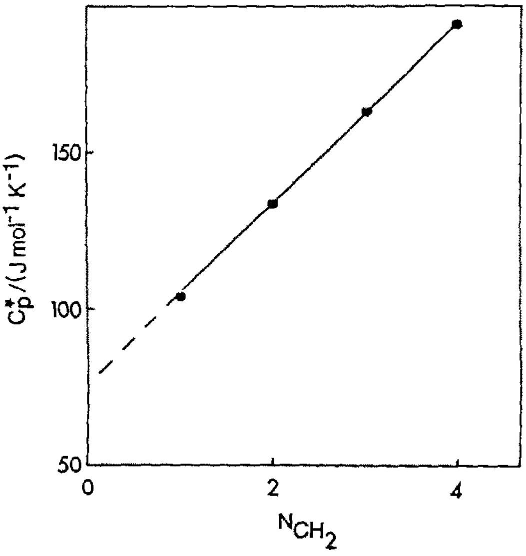

Fig. 1. Molar heat capacity values of α,ω-dibromoalkanes at 298.15 K versus number of methylene groups in the alkane chain N_{CH_2}.

we find that the bromides have an average C_p^* value that is 3.34 J K^{-1} mol^{-1} higher than the corresponding chlorides. The average value of the iodides is 2.39 J K^{-1} mol^{-1} higher than the corresponding bromine compounds. From these values we can obtain the group parameter value of iodine atom, $\phi(I) = 37.93 + 2.39 = 40.32$ J K^{-1} mol^{-1}, which is close to that reported by Missenard (40.38 J K^{-1} mol^{-1}). Similarly, $\phi(Cl) = 37.93 - 3.34 = 34.59$ J K^{-1} mol^{-1} which is in fair agreement with that reported by Chueh and Swanson using the group contribution method (36 J K^{-1} mol^{-1}).

Estimation of molar heat capacity

Very few accurate molar heat capacity values are currently available for halogenated compounds. It is thus important to develop empirical methods that apply to the estimation of such data. As stated earlier [18], estimation methods applicable for liquid heat capacities fall into four categories: theoretical, group contribution, corresponding states and Watson's thermodynamic cycle [17, 19]. In group contribution methods, we assume that various groups in a molecule contribute a definite value to the total molar heat capacity that is independent of other groups present. Many authors [8, 14–16, 20–26] have proposed values for different molecular groups to estimate constant-pressure liquid heat capacities. These methods usually have an error around of ±5% (Table 9). For halogenated compounds in particular, this may be due to the lack of experimental data.

Using the group parameter values $\phi(Y)$ of CH_2, Cl, Br and I (28.42, 34.59, 37.93 and 40.32 J K^{-1} mol^{-1}, respectively), we can calculate the group parameter value for the CH_3 group $\phi(CH_3)$ as follows. For straight-chain alkyl monohalogen compounds $CH_3(CH_2)_nX$ where $n = 0, 1, 2, \ldots$

$$\phi(CH_3) = C_p^*(CH_3(CH_2)_nX) - n\phi(CH_2) - \phi(X)$$

From this simple calculation one can obtain $\phi(CH_3)$ as 39.84 ± 0.21 J K^{-1} mol^{-1}.

Table 9 compares the Missenard and Chueh–Swanson calculated values with those estimated by the present method; it can be seen that the present method gives more accurate predictions than the other methods.

In conclusion, constant-pressure heat capacities were determined for 44 halogen hydrocarbons at 298.15 K and 308.15 K and atmospheric pressure from calorimetric measurements. It was shown that C_p values for the studied compounds increase linearly with the number of CH_2 groups present. On the basis of these results, the group contributions of the individual groups to the C_p values were determined. The C_p values can be calculated with sufficient accuracy by the group contribution method proposed here, knowing the chemical structure of the molecule.

TABLE 9

Comparison of experimental and calculated values estimated by different methods at 298.15 K

Compound	Molar heat capacity C_p^* (J mol^{-1} K^{-1})						
	Exp.	Missenard method		Chueh–Swanson method		Present method[b]	
		C_p^*	Err. (%)[a]	C_p^*	Err. (%)[a]	C_p^*	Err. (%)[a]
Chloro-compounds							
$ClCH_2Cl$	100.9	87.7	−13.1	102.4	1.5	97.6	−3.3
$Cl(CH_2)_2Cl$	129.4	115.9	−10.4	132.8	2.6	126.0	−2.6
$Cl(CH_2)_3Cl$	157.0	144.2	−8.2	163.2	3.9	154.4	−1.6
$Cl(CH_2)_4Cl$	184.0	172.4	−6.3	193.6	5.2	182.9	−0.6
$Cl(CH_2)_5Cl$	213.4	200.7	−6.0	224.0	5.0	211.3	−1.0
$CH_3(CH_2)_2Cl$	132.2	127.9	−3.3	133.2	0.8	131.3	−0.7
$CH_3(CH_2)_3Cl$	158.9	156.1	−1.8	163.6	3.0	159.7	0.5
$CH_3(CH_2)_4Cl$	187.7	184.3	−1.8	194.0	3.4	188.1	0.2
$CH_3(CH_2)_5Cl$	216.2	212.6	−1.7	224.4	3.8	216.5	0.2
$CH_3(CH_2)_6Cl$	245.4	240.8	−1.9	254.8	3.8	245.0	−0.2
$CH_3(CH_2)_7Cl$	274.7	269.0	−2.1	285.6	4.0	273.4	−0.5
Bromo-compounds							
$BrCH_2Br$	104.1	100.2	−3.7	106.4	2.2	104.3	0.2
$Br(CH_2)_2Br$	134.7	128.4	−4.7	136.8	1.6	132.7	−1.5
$Br(CH_2)_3Br$	163.7	156.7	−4.3	167.2	2.1	161.1	−1.6
$Br(CH_2)_4Br$	191.2	184.9	−3.3	197.6	3.3	189.5	−0.9
CH_3CH_2Br	105.8	105.9	0.1	105.2	−0.6	106.2	1.0
$CH_3(CH_2)_2Br$	134.6	134.1	−0.4	135.6	0.7	134.6	0.0
$CH_3(CH_2)_3Br$	162.2	162.3	0.1	166.0	2.3	163.0	0.5
$CH_3(CH_2)_4Br$	191.0	190.6	−0.2	196.4	2.8	191.5	0.2
$CH_3(CH_2)_5Br$	219.7	218.8	−0.4	226.8	3.2	219.9	0.1
$CH_3(CH_2)_6Br$	247.9	247.0	−0.4	257.2	3.8	248.3	0.2
Iodo-compounds							
ICH_2I	112.8	109.0	−3.4	102.4	−9.2	109.2	−3.2
$I(CH_2)_3I$	169.2	165.5	−2.2	163.2	−3.5	166.0	−1.9
CH_3I	82.0	82.0	0.0	72.8	−11.2	80.2	−2.2
CH_3CH_2I	109.7	110.2	0.5	103.2	−5.9	108.6	−1.0
$CH_3(CH_2)_2I$	136.2	138.5	1.7	133.6	−1.9	137.1	0.6
$CH_3(CH_2)_3I$	164.5	166.7	1.3	164.0	−0.3	165.5	0.6
$CH_3(CH_2)_4I$	193.6	195.0	0.7	194.4	0.4	193.9	0.2
$CH_3(CH_2)_5I$	222.5	223.2	0.3	224.8	1.0	222.3	0.1
$CH_3(CH_2)_6I$	251.8	251.5	−0.1	255.2	1.4	250.7	0.4

[a] Error (%) = (estimated value − exp. value) × 100/exp. value.

[b] These values were calculated using the group parameter values of CH_2, Cl, Br, I and CH_3 as 28.42, 34.59, 37.93, 40.32 and 39.84 J mol^{-1} K^{-1}, respectively.

ACKNOWLEDGEMENT

This work was carried out at the Thermochemistry Laboratory Chemical Center, University of Lund, Sweden. I am grateful to Professor Ingemar Wadsö and Professor Gerd Olofsson for their valuable discussions.

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