Vapor Pressure of Selected Organic Iodides

Michal Fulem,*[,†,‡] Květoslav Růžička,[†] Pavel Morávek,[†,‡] Jiří Pangrác,[‡] Eduard Hulicius,[‡] Boris Kozyrkin,[§] and Valery Shatunov[§]

Department of Physical Chemistry, Institute of Chemical Technology, Prague, Technická 5,
CZ-166 28 Prague 6, Czech Republic, Department of Semiconductors, Institute of Physics, Academy of Sciences of the Czech Republic, v.v.i., Cukrovarnická 10, 162 00 Prague 6, Czech Republic, and ALKYL, dom 3, str 1. proezd 4807, Zelenograd, Moscow, 124489, Russia

Vapor pressures of four organic iodides, 1-iodo-2-methylpropane (CAS Registry No. 513-38-2), 1-iodo-3-methylbutane (CAS Registry No. 541-28-6), 1-iodohexane (CAS Registry No. 638-45-9), and iodocyclohexane (CAS Registry No. 626-62-0), were measured using the static method in the technologically important temperature range (254 to 308) K. The experimental data were fitted with the Clarke and Glew equation. To our knowledge, this is the first time that vapor-pressure measurements for 1-iodohexane and iodocyclohexane are reported in the given temperature range. For 1-iodo-2-methylpropane and 1-iodo-3-methylbutane, the present measurements update the only available literature data originating from the year 1895.

Introduction

Organic iodides are commonly used in organic and organometallic chemistry as alkylating agents because of the easy formation and cleavage of the C−I bond. An overview of the literature sources reporting vapor-pressure data for 1-iodo-2-methylpropane, 1-iodo-3-methylbutane, 1-iodohexane, and iodocyclohexane given in Table 1 reveal that only fragmentary vapor-pressure data obtained in the studies devoted to the synthesis or correlations were published to date. Therefore, in this work, we report precise vapor-pressure data for these iodides in the temperature range (254 to 308) K.

Experimental Section

Materials. All of the studied iodides were supplied by Alkyl (Moscow, Russia) in sealed containers with copper pieces as a stabilizer. According to the manufacturer's NMR spectra, the mole fraction of organic impurities did not exceed $1.5 \cdot 10^{-3}$; according to the manufacturer's inductively coupled plasma (ICP) spectroscopy, the total mass fraction of metal impurities was below $1 \cdot 10^{-5}$. The thorough degassing was performed by a multistage vacuum distillation as described in detail in ref 1.

Apparatus and Procedure. Vapor pressures of the less volatile iodides, 1-iodohexane and iodocyclohexane, were determined using the static method with a newly constructed apparatus internally denoted as STAT6. The apparatus is schematically shown in Figure 1. It is constructed of stainless steel internally electrochemically polished tubing with ConFlat DN 16 CF and VCR connections and all-metal, pneumatically operated, angle valves VAT series 57 (VAT Vacuumvalves AG, Switzerland) for UHV. The pressure is measured simultaneously by two capacitance diaphragm absolute gauges MKS Baratron 690A01TRA and MKS Baratron 690A11TRA (MKS Instruments Inc., USA). Their measuring upper limits are (133 and 1333) Pa, respectively. The temperature of the pressure sensors is kept at $T =$ 318 K by an internal temperature controller. Calibrations of the pressure gauges at 318 K performed by the manufacturer at 11 equally spaced pressures from (0 to 130) Pa and (0 to 1300) Pa, respectively, with a maximum relative deviation of 0.03 %, are traceable to the National Institute of Standards and Technology (NIST). Additional calibrations focusing on the beginning of a pressure span were performed in the Czech Metrology Institute. The resulting relative uncertainty of the pressure reading is less than 0.05 %, which is the uncertainty stated by the manufacturer. The pressure readings from both pressure gauges in the overlapping pressure range coincide within the resolution of the model 690A11TRA, that is, 0.01 Pa.

The pressure gauges are connected to a stainless steel container with the measured material immersed in a Lauda RK 8 CP liquid bath thermostat that allows adjustment of the sample temperature in the temperature range from 233 K up to 473 K with stability better than 0.02 K. The sample temperature is measured by a platinum resistance thermometer Burns Engineering 12001-A-12-6-2-A in a four-wire connection calibrated by the manufacturer at the ice point and/or by comparison to a standard platinum resistance thermometer (SPRT). This SPRT was calibrated to the ITS-90, and its calibration was traceable to NIST. The uncertainty of the measurement of the sample temperature is less than 0.02 K, which is insignificant in the pressure range investigated in this work.

The tubing between the cell and the pressure gauges is placed in an insulated box thermostatted at a temperature higher than that of the sample to avoid condensation of its vapor. The box is thermostatted by using air convection forced by means of ventilators and is controlled to ± 0.2 K by a proportional−integral−derivative (PID) temperature regulator Eurotherm 2600 connected to a Pt100 thermometer.

The vacuum pump used to evacuate the system between the measuring cycles is a turbomolecular pump Pfeiffer vacuum TSH071 (Pfeiffer vacuum GmbH, Germany). The primary vacuum is ensured by a scroll vacuum pump Edwards XDS5 (Edwards Ltd., UK). The use of these vacuum pumps assures an oil-free pumping that significantly decreases the adsorption of measured samples caused by oil film that is formed when

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* Corresponding author. E-mail: michal.fulem@vscht.cz.

[†] Institute of Chemical Technology.

[‡] Institute of Physics, Academy of Sciences of the Czech Republic.

[§] ALKYL.

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Table 1. Overview of the Literature Vapor Pressure Data for the Studied Iodides[a]

ref	N[b]	$(T_{min} - T_{max})$/K	$(p_{min} - p_{max})$/kPa	note
1-Iodo-2-methylpropane				
Timmermans and Delcourt[10]	1	393.15	101.325	synthesis
Vogel[11]	1	392.65	102.792	synthesis
Stull[4]	S[c]	256.15 to 393.55	0.133 to 101.325	based on book by Anschütz and Keitter[5]
Franzen[12]	1	393.15 to 394.15	101.325	synthesis
Broadbent et al.[13]	1	321.15 to 322.15	7.333	synthesis
1-Iodo-3-methylbutane				
Stull[4]	S	270.65 to 421.35	0.133 to 101.325	based on book by Anschütz and Keitter[5]
Afanas'ev et al.[14]	1	422.15 to 423.15	101.325	synthesis
Hajipour et al.[15]	1	416.15 to 417.15	101.325	synthesis
1-Iodohexane				
Vogel[11]	2	318.71 to 453.15	0.533 to 103.192	synthesis
Mumford and Phillips[16]	1	349.65	3.066	synthesis
Franzen[12]	1	453.15 to 455.15	101.325	synthesis
Cavanna[17]	1	319.15	0.533	synthesis
Li and Rossini[18]	S	331.45 to 485.05	1.333 to 200	correlation
LeFevre and Orr[19]	1	316.15	0.333	synthesis
Geiseler et al.[20]	1	333.15	1.700	synthesis
Ogata and Aoki[21]	1	357.15	4.800	synthesis
Castro and Selve[22]	1	337.17	1.900	synthesis
Ciuhandu and Tirnaveanu[23]	1	337.15	1.867	synthesis
Hajipour et al.[15]	1	356.15 to 358.15	4.800	synthesis
Iodocyclohexane				
Stone and Schechter[24]	1	321.15 to 322.65	0.533	synthesis
Kornblum et al.[25]	1	338.15	1.467	synthesis
Forsman and Lipkin[26]	1	358.15 to 363.15	4.133	synthesis
Forsman and Lipkin[26]	1	368.15 to 370.15	6.133	synthesis
Brennan and Ubbelohde[27]	4	358.45 to 408.15	3.800 to 22.118	isoteniscope, unc. 0.2 K, 40 Pa
Lauwers et al.[28]	1	345.15	2.000	synthesis
Olah et al.[29]	1	341.15 to 342.15	1.333	synthesis
Morita et al.[30]	1	363.15 to 364.15	4.133	synthesis
Olah et al.[31]	1	311.15	0.200	synthesis
Imamoto et al.[32]	1	353.15	2.400	synthesis
Lecea et al.[33]	1	453.15 to 456.15	101.325	synthesis

[a] Literature data published prior to 1928 are not included in the table. [b] N stands for the number of experimental points. [c] S stands for smoothed data. Such data cannot a priori be used for further statistical treatment.

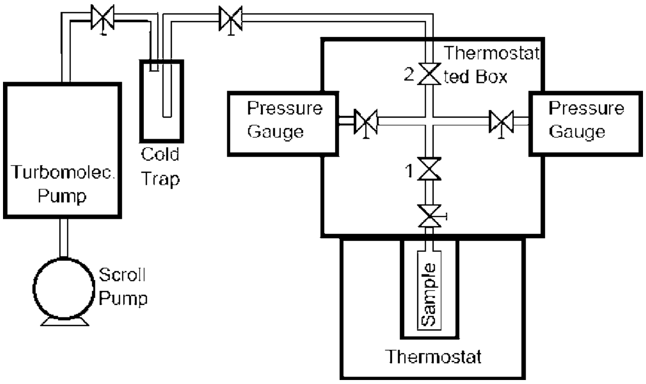

Figure 1. Static apparatus STAT 6 for the measurement of vapor pressure. Valves 1 and 2 are computer-controlled and take control of the measuring procedure.

rotary and/or diffusion pumps are used. A cold trap cooled down to 220 K by an electronic cooler (vapor-compression refrigeration device) is placed between the measuring system and the turbomolecular pump.

Prior to the measurement of vapor pressure, the apparatus is checked for tightness by an MKS PICO helium leak detector (MKS Instruments Inc., USA). The apparatus is evacuated between individual measurement cycles to a pressure of about 10^{-5} Pa. A computer using the Agilent VEE program monitors the temperature and pressure of the sample and controls the measuring procedure (temperature and valve control).

The performance of the STAT6 apparatus was checked by the measurement with naphthalene, which is recommended for calibrating vapor-pressure apparatuses.[2] The agreement with the recommended data[2] was within the uncertainty of the vapor-pressure measurements with the STAT6 apparatus, which is adequately described by the expression $\sigma(p/\text{Pa}) = 0.005(p/\text{Pa}) + 0.05$.

Vapor-pressure measurements of more volatile idodides, 1-iodo-2-methylpropane and 1-iodo-3-methylbutane, were performed using the static method with an apparatus internally denoted as STAT7. The apparatus and measuring procedure were previously described in detail.[1] The pressure is measured by a capacitance diaphragm absolute gage MKS Baratron 631A12TBEM (MKS Instruments Inc., USA). Its measuring upper limit is 13332 Pa, and the uncertainty is 0.25 % of the reading as stated by the manufacturer. The sample temperature is measured by a platinum resistance thermometer Burns Engineering 12001-A-12-6-2-A in a four-wire connection. The uncertainty of the temperature measurements is estimated to be less than 0.02 K. The uncertainty of the vapor-pressure measurements with the STAT 7 apparatus in the pressure range investigated is the same as with the STAT6 apparatus, that is, $\sigma(p/\text{Pa}) = 0.005(p/\text{Pa}) + 0.05$. All temperatures reported in this work are based on the international temperature scale ITS-90.

Results and Discussion

The vapor-pressure measurements were carried out in the temperature interval (254 to 308) K in which all of the studied iodides were liquids. The experiments were performed by varying the temperature at random to detect systematic errors caused by insufficient degassing of the sample. The measure-

Table 2. Experimental Vapor Pressures for 1-Iodo-2-methylpropane, 1-Iodo-3-methylbutane, 1-Iodohexane, and Iodocyclohexane

1-iodo-2-methylpropane			1-iodo-3-methylbutane			1-iodohexane			iodocyclohexane		
T/K	p/Pa	Δp^a/Pa	T/K	p/Pa	Δp^a/Pa	T/K	p/Pa	Δp^a/Pa	T/K	p/Pa	Δp^a/Pa
258.35	233.12	0.19	253.70	38.50	−0.03	258.18	6.85	0.00	258.17	5.26	0.01
258.35	233.13	0.20	253.68	38.32	−0.14	258.18	6.85	0.00	258.17	5.27	0.01
258.35	232.99	0.05	253.67	38.27	−0.16	258.17	6.84	0.00	258.17	5.25	0.00
263.70	340.51	0.25	258.62	58.03	0.43	263.17	10.90	0.00	263.17	8.29	−0.02
263.70	340.03	−0.24	258.62	57.89	0.29	263.17	10.90	0.01	263.17	8.30	−0.01
268.37	466.35	−0.83	268.98	127.59	0.13	263.17	10.90	0.00	263.17	8.29	−0.01
268.37	466.29	−0.89	269.10	127.97	−0.61	268.17	16.99	−0.02	268.17	12.85	−0.03
273.31	645.06	0.33	273.61	178.10	0.18	268.17	17.01	0.01	268.17	12.85	−0.02
273.31	644.61	−0.13	273.61	178.27	0.34	268.17	17.00	0.00	268.17	12.86	−0.01
278.35	883.59	−0.22	273.61	178.42	0.50	273.65	27.09	0.00	273.65	20.39	0.01
278.35	884.16	0.35	278.58	250.89	−0.20	273.65	27.07	−0.02	273.65	20.37	0.00
278.35	882.43	−1.38	278.56	250.40	−0.35	273.65	27.07	−0.01	278.15	29.28	0.03
283.39	1196.2	0.0	278.57	250.63	−0.29	278.15	39.10	0.04	278.15	29.27	0.01
283.39	1196.9	0.6	283.56	348.82	−1.05	278.15	39.09	0.03	283.15	43.14	0.09
283.39	1196.9	0.6	283.55	348.61	−1.04	283.15	57.71	0.00	283.15	43.08	0.03
288.35	1595.3	2.4	283.55	348.64	−1.00	283.15	57.69	−0.02	288.15	62.39	0.01
288.35	1594.9	2.0	288.52	482.06	1.27	288.15	83.99	0.08	288.15	62.38	0.00
293.27	2093.7	0.5	288.53	482.57	1.48	288.15	83.95	0.04	293.15	89.05	−0.02
293.27	2094.0	0.8	288.54	482.49	1.10	293.15	120.13	−0.02	293.15	89.05	−0.02
298.25	2731.6	0.4	293.57	655.14	−1.28	293.15	120.11	−0.05	298.15	125.39	−0.04
298.25	2732.0	0.7	293.55	655.76	0.13	298.15	169.45	−0.13	298.15	125.42	−0.01
298.25	2731.8	0.5	293.55	655.72	0.10	298.15	169.47	−0.11	303.15	174.23	−0.09
303.23	3525.6	−2.9	298.43	874.96	−1.07	303.15	235.94	−0.10	303.15	174.30	−0.02
303.23	3524.5	−4.1	298.44	875.35	−1.19	303.15	235.95	−0.09	308.16	239.38	−0.03
			298.44	875.62	−0.91	308.15	324.48	0.17	308.16	239.44	0.03
			303.29	1157.1	0.0	308.15	324.38	0.06	308.16	239.44	0.03
			303.29	1158.6	1.4	308.15	324.50	0.18			
			303.29	1159.7	2.6						

[a] $\Delta p = p - p_{\mathrm{calcd}}$, where p_{calcd} is calculated from the Clarke and Glew eq 1 with parameters given in Table 3.

Table 3. Parameters of Clarke and Glew Equation 1 at the Reference Temperatures $\theta = 298.15$ K and Pressure $p^0 = 10^5$ Pa

compound	$(T_{\min} - T_{\max})$ / K	$\Delta_l^g G_m^0$ / J·mol^{-1}	$\Delta_l^g H_m^0$ / J·mol^{-1}	$\Delta_l^g C_{p,m}^0$ / J·K^{-1}·mol^{-1}	σ^a / Pa	$T_{\mathrm{nbp}}{}^b$ / K
1-iodo-2-methylpropane	258 to 303	8938.25 ± 0.82	38766.92 ± 27.37	−36.56 ± 1.36	1.40	392.92
1-iodo-3-methylbutane	254 to 303	11784.67 ± 2.19	43183.17 ± 68.70	−33.59 ± 3.06	0.97	417.22
1-iodohexane	258 to 308	15814.90 ± 0.37	49887.15 ± 10.72	−71.53 ± 0.60	0.07	460.73
iodocyclohexane	258 to 308	16562.38 ± 0.79	49613.17 ± 23.48	−56.25 ± 1.31	0.03	469.18

[a] σ is the standard deviation of the fit defined as $\sigma = [\sum_{i=1}^{n}(\Delta p)_i^2/(n - m)]^{1/2}$, where Δp is the difference between the experimental and the smoothed values, n is the number of experimental points used in the fit, and m is the number of adjustable parameters of Clarke and Glew eq 1. [b] T_{nbp} is the normal boiling temperature calculated from Clarke and Glew eq 1.

ments were performed repeatedly at selected temperatures. When the pressure did not change with the number of measuring cycles, the sample was considered completely degassed, and the final set of data was recorded. At least two experimental points were obtained for each temperature.

The experimental data on vapor pressure listed in Table 2 were fitted with the Clarke and Glew equation[3]

$$R \ln\left(\frac{p}{p^0}\right) = -\frac{\Delta_l^g G_m^0(\theta)}{\theta} + \Delta_l^g H_m^0(\theta)\left(\frac{1}{\theta} - \frac{1}{T}\right) + \Delta_l^g C_{p,m}^0(\theta)\left[\left(\frac{\theta}{T}\right) - 1 + \ln\left(\frac{T}{\theta}\right)\right] \quad (1)$$

where p is the vapor pressure, p^0 is a selected reference pressure, θ is a selected reference temperature, R is the molar gas constant ($R = 8.314472$ J·K^{-1}·mol^{-1}), $\Delta_l^g G_m^0$ is the difference in molar Gibbs energy between the gaseous and the liquid phase at the selected reference pressure (the gaseous phase is assume to be an ideal gas at the pressure p^0), $\Delta_l^g H_m^0$ is the vaporization enthalpy, and $\Delta_l^g C_{p,m}^0$ is the difference between the heat capacities of the ideal gas and of the liquid phase. Given the temperature range studied, the use of the Clarke and Glew eq 1 with three parameters is adequate. The advantage of this equation lies in a physical significance of the fitted parameters. The parameters of the Clarke and Glew eq 1 together with the standard deviation of the fit, σ, and calculated normal boiling temperatures, T_{nbp}, are presented in Table 3. Figure 2 shows the relative deviations of the experimental vapor pressure data for all of the studied iodides from the smoothed values obtained from eq 1. The relative deviations do not exceed 0.25 % for 1-iodo-2-methylpropane, 1-iodohexane, and iodocyclohexane and 0.75 % for 1-iodo-3-methylbutane.

The comparison of the vapor-pressure data from this work with the literature results is shown in Figure 3. In the studied temperature interval only smoothed data for 1-iodo-2-methylpropane and 1-iodo-3-methylbutane reported by Stull[4] were found in the literature. Stull's smoothed data were obtained from the data published in the book by Anschütz and Keitter[5] in 1895 (we were unable to obtain original data points from this book). The relative deviations range from (23 to 33) % for 1-iodo-2-methylpropane and from (7.0 to 7.5) % for 1-iodo-3-methylbutane in the temperature range studied.

As the normal boiling temperature, T_{nbp}, is one of the basic characteristics of a compound used as input in many correlations and estimation methods, T_{nbp} were calculated using eq 1 (see Table 3). Given the length of extrapolation, these values compare satisfactorily with most of T_{nbp} that can be identified in Table 1. The properties derived from the vapor-pressure data, the standard molar enthalpy of vaporization at $T = 298$ K,

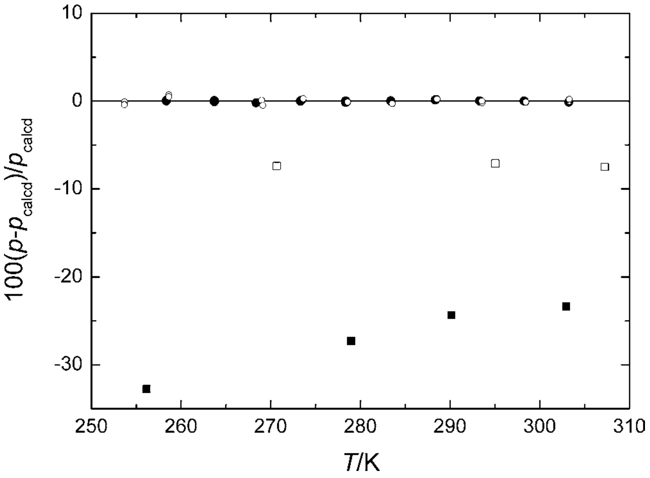

Figure 2. Comparison of vapor pressures p for 1-iodo-2-methylpropane and 1-iodo-3-methylbutane obtained in this work with the literature values. $p_{\rm calcd}$ is obtained from Clarke and Glew eq 1. ●, this work (1-iodo-2-methylpropane); ○, this work (1-iodo-3-methylbutane); ■, Stull[4] (1-iodo-2-methylpropane); □, Stull[4] (1-iodo-3-methylbutane).

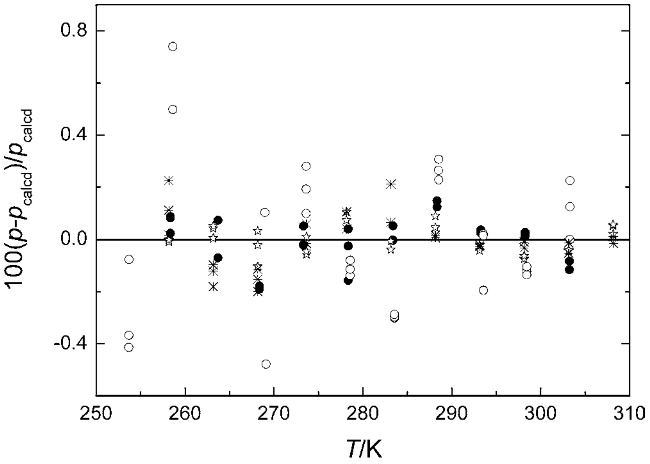

Figure 3. Comparison of experimental vapor pressures p for all of the studied iodides from this work with smoothed values $p_{\rm calcd}$ obtained from Clarke and Glew eq 1. ●, 1-iodo-2-methylpropane; ○, 1-iodo-3-methylbutane; ☆, 1-iodohexane; ∗, iodocyclohexane.

$\Delta_{\rm l}^{\rm g}H_{\rm m}^0$(298.15 K), and $\Delta_{\rm l}^{\rm g}C_{p,{\rm m}}^0(298.15\ {\rm K}) = C_{p,{\rm m}}^{\rm g,0}(298.15\ {\rm K}) - C_{p,{\rm m}}^{\rm l}(298.15\ {\rm K})$, are compared with the literature values in Table 4. Values of $\Delta_{\rm l}^{\rm g}H_{\rm m}^0$(298.15 K) obtained in this work for 1-iodo-2-methylpropane and 1-iodohexane are in excellent agreement with those determined calorimetrically by Wadsö.[6] Values of $\Delta_{\rm l}^{\rm g}C_{p,{\rm m}}^0$(298.15 K) compare reasonably with values obtained from calorimetric measurements of $C_{p,{\rm m}}^{\rm l}$(298.15 K)[7,8] and $C_{p,{\rm m}}^{\rm g,0}$(298.15 K) estimated by Benson method.[9]

Conclusions

New vapor-pressure data for four organic iodides, 1-iodo-2-methylpropane, 1-iodo-3-methylbutane, 1-iodohexane, and iodocyclohexane, were determined using the static method in the temperature range (254 to 308) K. The present measurements significantly extend and update the fragmentary volatility data available in the literature. The vapor-pressure data for 1-iodo-2-methylpropane and 1-iodohexane are consistent with high-precision vaporization enthalpies obtained calorimetrically by Wadsö.[6]

Table 4. Comparison of $\Delta_{\rm l}^{\rm g}H_{\rm m}^0$(298.15 K) and $\Delta_{\rm l}^{\rm g}C_{p,{\rm m}}^0$(298.15 K) Derived from the Vapor-Pressure Data from This Work with the Literature Values[a]

ref	$\Delta_{\rm l}^{\rm g}H_{\rm m}^0$(298.15 K) kJ·mol^{-1}	$\Delta_{\rm l}^{\rm g}C_{p,{\rm m}}^0$(298.15 K) J·K^{-1}·mol^{-1}	method
	1-Iodo-2-methylpropane		
this work	38.8	−36.6	VP[b]
Stull[4]	40.9	−28.0	VP[b,c]
Wadsö[6]	38.83		C[d]
Kolská et al.[34]	38.5		GCEM[e]
Shehatta[8]		−57.1[f]	C[d]
	1-Iodo-3-methylbutane		
this work	43.2	−33.6	VP[b]
Stull[4]	43.0	−36.1	VP[b,c]
Chickos et al.[35]	42.22		CGC[g]
Kolská et al.[34]	43.3		GCEM[e]
	1-Iodohexane		
this work	49.9	−71.5	VP[b]
Wadsö[6]	49.75		C[d]
Kolská et al.[34]	50.5		GCEM[e]
Shehatta[8]		−67.3[f]	C[d]
Bolotnikov and Neruchev[7]		−62.9[f]	C[d]
	Iodocyclohexane		
this work	49.6	−56.3	VP[b]
Chickos et al.[35]	48.32		CGC[g]
Kolská et al.[34]	48.8		GCEM[e]

[a] $\Delta_{\rm l}^{\rm g}H_{\rm m}^0$(298.15 K) is the standard molar vaporization enthalpy at T = 298.15 K; $\Delta_{\rm l}^{\rm g}C_{p,{\rm m}}^0(298.15\ {\rm K}) = C_{p,{\rm m}}^{\rm g,0}(298.15\ {\rm K}) - C_{p,{\rm m}}^{\rm l}(298.15\ {\rm K})$, where $C_{p,{\rm m}}^{\rm g,0}$(298.15 K) and $C_{p,{\rm m}}^{\rm l}$(298.15 K) are the heat capacities of ideal gas and liquid at T = 298.15 K, respectively. [b] VP stands for data calculated from vapor pressures. [c] Vapor pressure fitted to the Clarke and Glew equation in this work. [d] C stands for calorimetric determination. [e] GCEM stands for group contribution estimation method. [f] $C_{p,{\rm m}}^{\rm g,0}$(298.15 K) was estimated by the Benson method.[9] [g] CGC stands for determination by correlation gas chromatography.

Literature Cited

(1) Pangrác, J.; Fulem, M.; Hulicius, E.; Melichar, K.; Šimeček, T.; Růžička, K.; Morávek, P.; Růžička, V.; Rushworth, S. A. Vapor pressure of germanium precursors. *J. Cryst. Growth* **2008**, *310*, 4720–4723.

(2) Růžička, K.; Fulem, M.; Růžička, V. Recommended Vapor Pressure of Solid Naphthalene. *J. Chem. Eng. Data* **2005**, *50*, 1956–1970.

(3) Clarke, E. C. W.; Glew, D. N. Evaluation of thermodynamic functions from equilibrium constants. *Trans. Faraday Soc.* **1966**, *62*, 539–547.

(4) Stull, D. R. Vapor Pressure of Pure Substances - Organic Compounds. *Ind. Eng. Chem.* **1947**, *39*, 517–540.

(5) Anschütz, H.; Keitter, E. *Die Destillation unter vermindertem Druck im Laboratorium*, 2nd ed.; Cohen: Bonn, 1895.

(6) Wadsö, I. Heats of Vaporization of Organic Compounds. 2. Chlorides Bromides and Iodides. *Acta Chem. Scand.* **1968**, *22*, 2438–2444.

(7) Bolotnikov, M. F.; Neruchev, Y. A. Temperature dependence of the thermophysical properties of 1-chlorohexane, 1-iodohexane, 1-iodoheptane, and 1-chlorononane at saturation condition. *J. Chem. Eng. Data* **2004**, *49*, 202–207.

(8) Shehatta, I. Heat-Capacity at Constant Pressure of Some Halogen Compounds. *Thermochim. Acta* **1993**, *213*, 1–10.

(9) Stein, S. E.; Brown, R. L. Structures and Properties Group Additivity Model. In *NIST Chemistry WebBook, NIST Standard Reference Database Number*, 69th ed.; Linstrom, P. J., Mallard, W. G., Eds.; NIST: Gaithersburg, MD, http://webbook.nist.gov (retrieved April 22, 2010).

(10) Timmermans, J.; Delcourt, Y. Work of the International Bureau of Physico-Chemical Standards. VI. Physical constants of twenty organic compounds. *J. Chim. Phys. Phys.-Chim. Biol.* **1934**, *31*, 85–124.

(11) Vogel, A. I. Physical properties and chemical constitution. VIII. Alkyl chlorides, bromides and iodides. *J. Chem. Soc.* **1943**, 636–647.

(12) Franzen, V. Eine Methode zum Austausch von Chlor oder Brom gegen Jod bei aliphatischen und aromatischen Verbindungen. *Chem. Ber.* **1954**, *87*, 1148–1154.

(13) Broadbent, H. S.; Burnham, W. S.; Sheeley, R. M.; Olsen, R. K. Novel heterotricyclic systems: 2,6-dioxa- and 2-oxa-6-thia-10-azatricyclo-[5.2.1.0^{4,10}decanes; 2,6-dioxa-11-azatricyclo[5.3.1.0^{4,11}undecane; and 9,13-dioxa-14-azatetracyclo[6.5.1.0.^{2,7}0^{11,14}tetradeca-2,4,6-triene (1a,b). *J. Heterocycl. Chem.* **1976**, *13*, 337–348.

(14) Afanas'ev, I. B.; Safronenko, E. D.; Katsobashvili, V. Y. Radical reaction of ethylene and tetrafluoroethylene with isopropyl halides. *Zh. Org. Khim.* **1966**, *2*, 423–426.
(15) Hajipour, A. R.; Mostafavi, M.; Ruoho, A. E. Iodination of alcohols using triphenylphosphine/iodine in ionic liquid under solvent-free conditions. *Org. Prep. Proced. Int.* **2009**, *41*, 87–91.
(16) Mumford, S. A.; Phillips, J. W. C. The Physical Properties of Some Aliphatic Compounds. *J. Chem. Soc.* **1950**, 75–84.
(17) Cavanna, R. Synthesis of the Racemic and Optically Active Forms of 10-Methylnonadecanoic Acid. *Acta Chem. Scand.* **1956**, *10*, 1527–1530.
(18) Li, J. C. M.; Rossini, F. D. Vapor pressures and boiling points of the 1-fluoroalkanes, 1-chloroalkanes, 1-bromoalkanes, and 1-iodoalkanes, C1 to C20. *J. Chem. Eng. Data* **1961**, *6*, 268–270.
(19) Le Fevre, R. J. W.; Orr, B. J. Molecular polarizability. The molar Kerr constants and dipole moments of twelve alkyl iodides. *J. Chem. Soc.* **1965**, 5349–5353.
(20) Geiseler, G.; Fruwert, J.; Schmidt, L.; Schwalbe, S. Influence of Chain Length on Integral Absorption of Unbranched Homologous Alkane Derivatives. *Spectrochim. Acta, Part A* **1968**, *A 24*, 1007–1012.
(21) Ogata, Y.; Aoki, K. Reaction of Alkyl Iodides with Peracetic Acid in Presence of Aromatic Compounds. *J. Org. Chem.* **1969**, *34*, 3974–3977.
(22) Castro, B.; Selve, C. Alkyloxy-Phosphonium Salts 0.1. Preparation, Stability and Reactivity of Tri-Dimethylamino-Alkyloxy-Phosphonium Salts Containing Primary Alkyl Groups. *Bull. Soc. Chim. Fr.* **1971**, 2296–2298.
(23) Ciuhandu, G.; Tirnaveanu, A. Decarbonylation reactions. III. Decarbonylation of formamide and some of its derivatives. *Rev. Roum. Chim.* **1971**, *16*, 1231–1235.
(24) Stone, H.; Schechter, H. Iodocyclohexane. *Org. Synth.* **1951**, *31*, 66–67.
(25) Kornblum, N.; Kelley, A. E.; Cooper, G. D. Chemistry of diazo compounds. III. Reduction of diazonium salts by phosphorous acid. *J. Am. Chem. Soc.* **1952**, *74*, 3074–3076.
(26) Forsman, J. P.; Lipkin, D. The reactions of phenyl esters of phosphorous acid with iodine. *J. Am. Chem. Soc.* **1953**, *75*, 3145–3148.
(27) Brennan, D.; Ubbelohde, A. R. Thermochemical evaluation of bond strengths in some carbon compounds. IV. Bond-strength differences based on the reaction: RI + HI−> RH + I_2, where R = *p*-methoxyphenyl and cyclohexyl. *J. Chem. Soc.* **1956**, 3011–3016.
(28) Lauwers, M.; Regnier, B.; Van Eenoo, M.; Denis, J. N.; Krief, A. Diphosphorus tetraiodide (P2I4). A valuable reagent for regioselective synthesis of iodo alkanes from alcohols. *Tetrahedron Lett.* **1979**, 1801–1804.
(29) Olah, G. A.; Welch, J. T.; Vankar, Y. D.; Nojima, M.; Kerekes, I.; Olah, J. A. Synthetic methods and reactions. 63. Pyridinium poly(hydrogen fluoride) (30% pyridine-70% hydrogen fluoride): a convenient reagent for organic fluorination reactions. *J. Org. Chem.* **1979**, *44*, 3872–81.
(30) Morita, T.; Yoshida, S.; Okamoto, Y.; Sakurai, H. Chlorotrimethylsilane/sodium iodide: a new reagent for conversion of alcohols into iodides. *Synthesis* **1979**, 379.
(31) Olah, G. A.; Husain, A.; Singh, B. P.; Mehrotra, A. K. Synthetic methods and reactions. 112. Synthetic transformations with trichloromethylsilane/sodium iodide reagent. *J. Org. Chem.* **1983**, *48*, 3667–3672.
(32) Imamoto, T.; Matsumoto, T.; Kusumoto, T.; Yokoyama, M. A convenient method for the preparation of alkyl iodides from alcohols. *Synthesis* **1983**, 460–461.
(33) Lecea, B.; Aizpurua, J. M.; Palomo, C. Reagents and synthetic methods 52. Silane reduction of carbonyl compounds in the presence of iodine. *Tetrahedron* **1985**, *41*, 4657–4665.
(34) Kolská, Z.; Růžička, V.; Gani, R. Estimation of the enthalpy of vaporization and the entropy of vaporization for pure organic compounds at 298.15 K and at normal boiling temperature by a group contribution method. *Ind. Eng. Chem. Res.* **2005**, *44*, 8436–8454.
(35) Chickos, J. S.; Hosseini, S.; Hesse, D. G. Determination of vaporization enthalpies of simple organic molecules by correlations of changes in gas chromatographic net retention times. *Thermochim. Acta* **1995**, *249*, 41–62.

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