

2.5.4 Chloroiodo- and Fluoroiodoalkanes

1-Chloro-2-iodoethane [624-70-4] $\text{C}_2\text{H}_4\text{ClI}$ MW = 190.41 579

Table 1. Experimental values with uncertainties.

T K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ $\text{kg} \cdot \text{m}^{-3}$	Ref.
288.43	2133.57 ± 0.60	1880-tho
288.58	2133.23 ± 0.60	1880-tho

Trifluoroiodomethane [2314-97-8] CF_3I MW = 195.91 580

$T_c = 396.44 \text{ K}$ [2000-dua/shi]

$\rho_c = 868.00 \text{ kg} \cdot \text{m}^{-3}$ [2000-dua/shi]

Table 1. Coefficients for the polynomial expansion equations. Standard deviations (see introduction): $\sigma_t = 3.2612 \cdot 10^{-1}$ (low temperature range), $\sigma_{c,w} = 4.4436$ (combined temperature ranges, weighted), $\sigma_{c,uw} = 1.2956$ (combined temperature ranges, unweighted).

Coefficient	$T = 301.02 \text{ to } 325.00 \text{ K}$ $\rho = A + BT + CT^2 + DT^3 + \dots$	$T = 325.00 \text{ to } 396.44 \text{ K}$ $\rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)]$ $[\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3 + D(T_c - T)^4]$
A	$9.03139 \cdot 10^2$	-2.45814
B	$1.26487 \cdot 10^1$	$1.58749 \cdot 10^{-1}$
C	$-2.96396 \cdot 10^{-2}$	$-2.87111 \cdot 10^{-3}$
D		$1.65491 \cdot 10^{-5}$

Table 2. Experimental values with uncertainties and deviation from calculated values.

T K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ $\text{kg} \cdot \text{m}^{-3}$	$\rho_{\text{exp}} - \rho_{\text{calc}}$ $\text{kg} \cdot \text{m}^{-3}$	Ref. (Symbol in Fig. 1)	T K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ $\text{kg} \cdot \text{m}^{-3}$	$\rho_{\text{exp}} - \rho_{\text{ca}}$ $\text{kg} \cdot \text{m}^{-3}$	Ref. (Symbol in Fig. 1)
301.02	2024.90 ± 2.00	-0.02	1999-dua/shi(□)	355.19	1676.70 ± 2.00	-2.23	1999-dua/shi(□)
307.13	1992.00 ± 2.00	-0.07	1999-dua/shi(□)	368.59	1552.10 ± 2.00	6.97	1999-dua/shi(□)
313.09	1958.20 ± 2.00	0.31	1999-dua/shi(□)	378.13	1438.80 ± 3.00	8.29	1999-dua/shi(□)
319.75	1917.10 ± 2.00	-0.11	1999-dua/shi(□)	386.59	1305.30 ± 3.00	-4.69	1999-dua/shi(□)
319.93	1915.50 ± 2.00	-0.57	1999-dua/shi(□)	390.30	1229.90 ± 4.00	-12.70	1999-dua/shi(□)
322.08	1902.80 ± 2.00	0.45	1999-dua/shi(□)	392.62	1173.00 ± 4.00	-14.53	1999-dua/shi(□)
326.03	1878.50 ± 2.00	1.94	1999-dua/shi(□)	394.26	1124.90 ± 4.00	-8.71	1999-dua/shi(□)
331.49	1843.50 ± 2.00	0.49	1999-dua/shi(□)	395.30	1070.50 ± 4.00	-12.13	1999-dua/shi(□)
334.74	1822.50 ± 2.00	-1.20	1999-dua/shi(□)	395.85	1020.30 ± 5.00	-20.42	1999-dua/shi ¹⁾
339.80	1793.60 ± 2.00	0.74	1999-dua/shi(□)	396.17	983.40 ± 5.00	-17.94	1999-dua/shi ¹⁾
340.83	1781.20 ± 2.00	-5.13	1999-dua/shi(□)	396.42	920.70 ± 5.00	-3.41	1999-dua/shi ¹⁾
344.14	1758.30 ± 2.00	-6.17	1999-dua/shi(□)				

¹⁾ Not included in Fig. 1.

cont.

Trifluoroiodomethane (cont.)

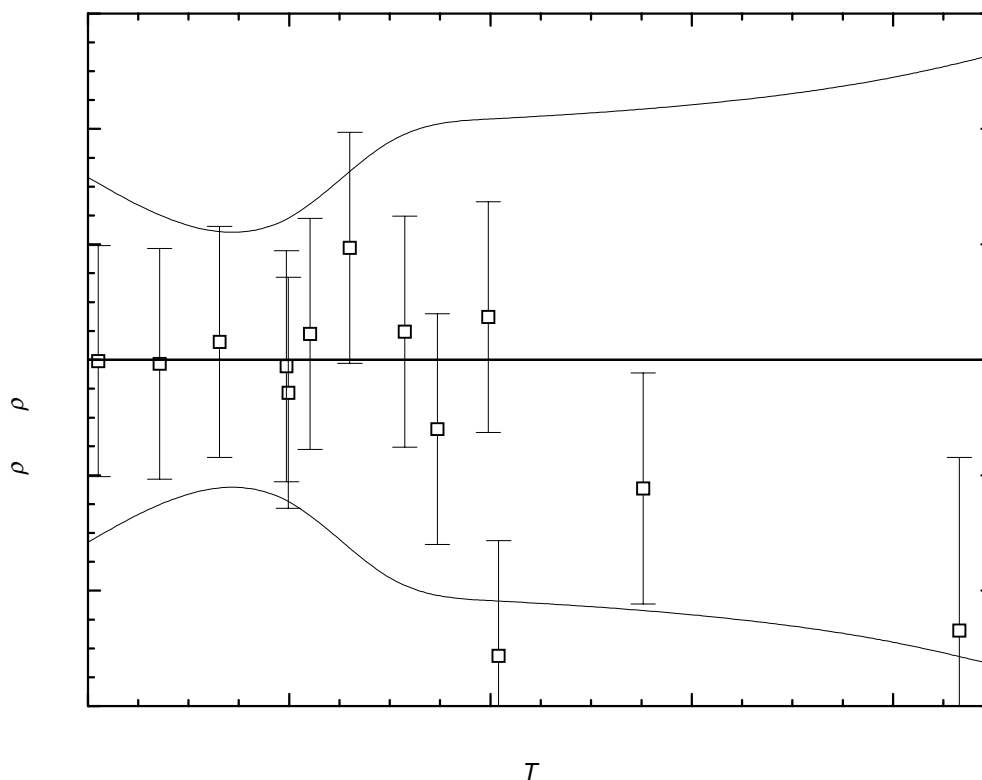


Fig. 1. The symbols show the deviation of the calculated from the experimental values from Table 2. The curves above and below the zero line indicate the calculated error region of the recommended values given in Table 3. The error bars represent the experimental errors. (Error bars smaller than the symbols are omitted for clarity of the figure.)

Table 3. Recommended values (fit to the reliable experimental values according to the equations

$$\rho = A + BT + CT^2 + DT^3 + \dots \text{ or } \rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)][\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3 + D(T_c - T)^4]$$

$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
300.00	2030.19 ± 3.16	340.00	1791.60 ± 4.17	380.00	1405.95 ± 4.87
310.00	1975.87 ± 2.17	350.00	1721.77 ± 4.27	390.00	1248.75 ± 5.28
320.00	1915.63 ± 2.13	360.00	1634.70 ± 4.41		
330.00	1851.93 ± 4.09	370.00	1529.19 ± 4.60		

Fluorodiiodomethane**[1493-01-2]****MW = 285.83****581****Table 1.** Fit with estimated B coefficient for 3 accepted points. Deviation $\sigma_w = 0.262$.

Coefficient	$\rho = A + BT$
<i>A</i>	4169.21
<i>B</i>	-3.300

Table 2. Experimental values with uncertainties and deviation from calculated values.

T K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ kg · m ⁻³	$\rho_{\text{exp}} - \rho_{\text{calc}}$ kg · m ⁻³	Ref.
<i>crystal</i>			
80.15	3640.0 ± 5.0		1936-ruf/bre
<i>liquid</i>			
253.75	3331.50 ± 2.00	-0.34	1936-ruf/bre
287.55	3220.60 ± 2.00	0.30	1936-ruf/bre
294.65	3196.90 ± 2.00	0.03	1936-ruf/bre

Table 3. Recommended values.

T K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ kg · m ⁻³
250.00	3344.2 ± 3.4
260.00	3311.2 ± 2.6
270.00	3278.2 ± 2.0
280.00	3245.2 ± 1.8
290.00	3212.2 ± 2.1
293.15	3201.8 ± 2.3
298.15	3185.3 ± 2.7

Pentafluoroiodoethane**[354-64-3]****MW = 245.92****582****Table 1.** Experimental values with uncertainties.

T K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ kg · m ⁻³	Ref.
273.15	2160.50 ± 3.00	1953-nod/gro
296.65	2071.80 ± 3.00	1953-nod/gro