

## 5.4 Aromatic Halohydrocarbons of General Formula $C_nH_{2n-6-(k+l)}A_kB_l$ (A,B - elements of halogen series)

**1-Bromo-2-chlorobenzene****[694-80-4]** **$C_6H_4BrCl$** **MW = 191.45****929****Table 1.** Fit with estimated B coefficient for 8 accepted points. Deviation  $\sigma_w = 0.423$ .

Coefficient	$\rho = A + BT$
A	2050.59
B	-1.350

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

$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref.	$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref.
259.00	$1701.60 \pm 1.00$	0.66	1980-vit/ber	276.80	$1676.80 \pm 1.00$	-0.11	1980-vit/ber
265.40	$1692.70 \pm 1.00$	0.40	1980-vit/ber	280.40	$1671.80 \pm 1.00$	-0.25	1980-vit/ber
268.80	$1688.00 \pm 1.00$	0.29	1980-vit/ber	285.00	$1665.40 \pm 1.00$	-0.44	1980-vit/ber
272.60	$1682.70 \pm 1.00$	0.12	1980-vit/ber	290.30	$1658.00 \pm 1.00$	-0.68	1980-vit/ber

**Table 3.** Recommended values.

$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$
250.00	$1713.1 \pm 1.6$
260.00	$1699.6 \pm 1.2$
270.00	$1686.1 \pm 1.0$
280.00	$1672.6 \pm 1.0$
290.00	$1659.1 \pm 1.2$
293.15	$1654.8 \pm 1.3$
298.15	$1648.1 \pm 1.5$

**1-Bromo-3-chlorobenzene****[108-37-2]** **$C_6H_4BrCl$** **MW = 191.45****930****Table 1.** Fit with estimated B coefficient for 2 accepted points. Deviation  $\sigma_w = 0.000$ .

Coefficient	$\rho = A + BT$
A	2026.11
B	-1.360

cont.

**1-Bromo-3-chlorobenzene** (cont.)**Table 2.** Experimental values with uncertainties and deviation from calculated values.

$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref.
293.15	$1627.40 \pm 0.50$	0.00	1949-dre/mar
298.15	$1620.60 \pm 0.50$	0.00	1949-dre/mar

**Table 3.** Recommended values.

$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$
290.00	$1631.7 \pm 0.5$
293.15	$1627.4 \pm 0.5$
298.15	$1620.6 \pm 0.5$

**1-Bromo-4-chlorobenzene**

[106-39-8]

 $C_6H_4BrCl$ 

MW = 191.45

931

**Table 1.** Fit with estimated B coefficient for 5 accepted points. Deviation  $\sigma_w = 1.449$ .

Coefficient	$\rho = A + BT$
A	2097.25
B	-1.510

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

$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref.
344.15	$1576.00 \pm 1.50$	-1.58	1924-sug-2
369.15	$1540.00 \pm 1.50$	0.17	1924-sug-2
390.15	$1508.00 \pm 1.70$	-0.12	1924-sug-2
411.15	$1476.00 \pm 1.70$	-0.41	1924-sug-2
428.15	$1454.00 \pm 2.00$	3.26	1924-sug-2

**Table 3.** Recommended values.

$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$
340.00	$1583.8 \pm 2.7$	380.00	$1523.4 \pm 2.1$	420.00	$1463.0 \pm 2.6$
350.00	$1568.7 \pm 2.5$	390.00	$1508.3 \pm 2.1$	430.00	$1447.9 \pm 2.8$
360.00	$1553.6 \pm 2.3$	400.00	$1493.2 \pm 2.2$		
370.00	$1538.5 \pm 2.2$	410.00	$1478.1 \pm 2.3$		

**Chloropentafluorobenzene****[344-07-0]** **$C_6ClF_5$** **MW = 202.51****932**

**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{c,w} = 3.0567 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 1.1948 \cdot 10^{-1}$  (combined temperature ranges, unweighted).

Coefficient	$T = 293.15 \text{ to } 490.00 \text{ K}$ $\rho = A + BT + CT^2 + DT^3 + \dots$
<i>A</i>	$2.57357 \cdot 10^3$
<i>B</i>	-5.42422
<i>C</i>	$1.11479 \cdot 10^{-2}$
<i>D</i>	$-1.18685 \cdot 10^{-5}$

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

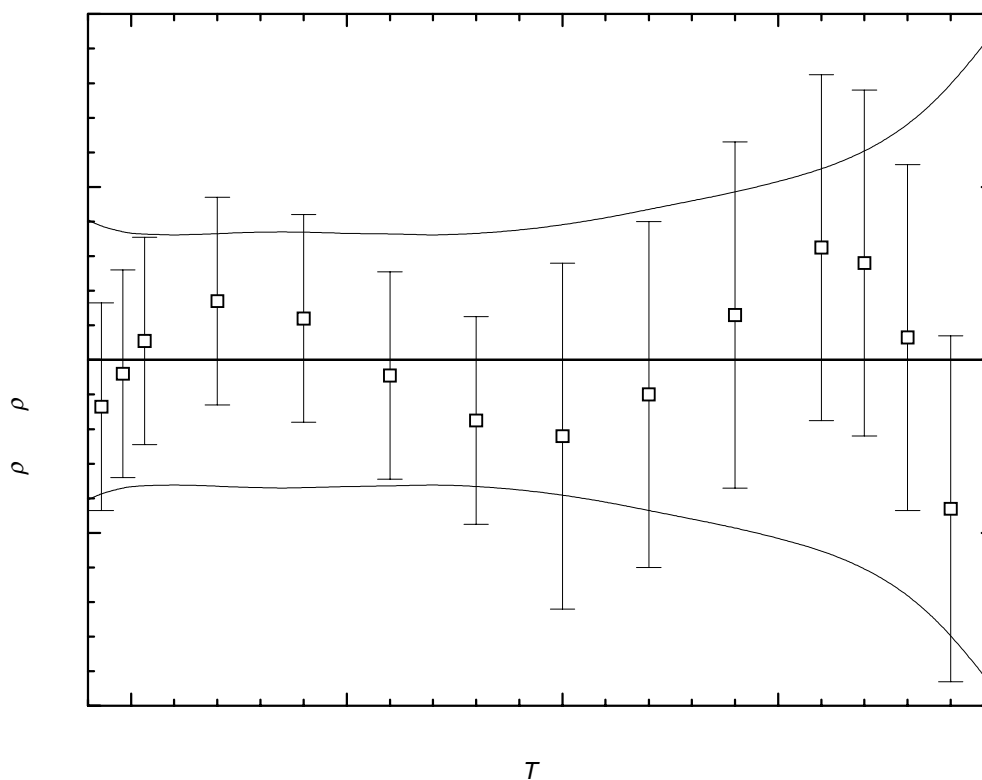
$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)
293.15	$1642.21 \pm 0.60$	-0.27	1974-hal/tow(□)	400.00	$1427.52 \pm 1.00$	-0.44	1974-hal/tow(□)
298.15	$1632.68 \pm 0.60$	-0.08	1974-hal/tow(□)	420.00	$1382.37 \pm 1.00$	-0.20	1974-hal/tow(□)
303.15	$1623.17 \pm 0.60$	0.11	1974-hal/tow(□)	440.00	$1334.40 \pm 1.00$	0.26	1974-hal/tow(□)
320.00	$1590.80 \pm 0.60$	0.34	1974-hal/tow(□)	460.00	$1282.74 \pm 1.00$	0.65	1974-hal/tow(□)
340.00	$1551.79 \pm 0.60$	0.24	1974-hal/tow(□)	470.00	$1255.09 \pm 1.00$	0.56	1974-hal/tow(□)
360.00	$1511.79 \pm 0.60$	-0.09	1974-hal/tow(□)	480.00	$1225.99 \pm 1.00$	0.13	1974-hal/tow(□)
380.00	$1470.52 \pm 0.60$	-0.35	1974-hal/tow(□)	490.00	$1195.13 \pm 1.00$	-0.86	1974-hal/tow(□)

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

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

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
290.00	$1648.62 \pm 0.81$	350.00	$1531.85 \pm 0.73$	430.00	$1358.77 \pm 0.92$
293.15	$1642.48 \pm 0.77$	360.00	$1511.88 \pm 0.73$	440.00	$1334.14 \pm 0.97$
298.15	$1632.76 \pm 0.74$	370.00	$1491.58 \pm 0.72$	450.00	$1308.60 \pm 1.03$
300.00	$1629.16 \pm 0.73$	380.00	$1470.87 \pm 0.73$	460.00	$1282.09 \pm 1.10$
310.00	$1609.80 \pm 0.72$	390.00	$1449.69 \pm 0.75$	470.00	$1254.53 \pm 1.20$
320.00	$1590.46 \pm 0.73$	400.00	$1427.96 \pm 0.78$	480.00	$1225.86 \pm 1.35$
330.00	$1571.06 \pm 0.74$	410.00	$1405.61 \pm 0.82$	490.00	$1195.99 \pm 1.58$
340.00	$1551.55 \pm 0.74$	420.00	$1382.57 \pm 0.87$	500.00	$1164.87 \pm 1.90$

cont.

**Chloropentafluorobenzene (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.)

**1,2,3-Trichlorotrifluorobenzene****[827-12-3]** **$C_6Cl_3F_3$** **MW = 235.42****933**

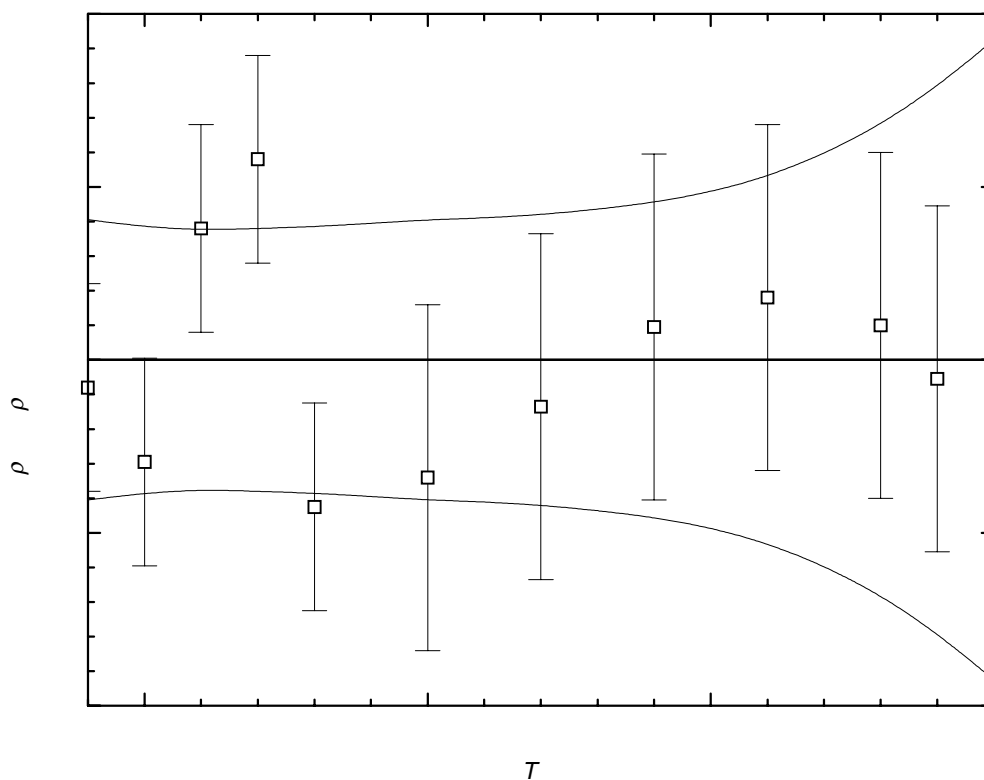
**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{c,w} = 6.1928 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 1.9553 \cdot 10^{-1}$  (combined temperature ranges, unweighted).

Coefficient	$T = 340.00 \text{ to } 490.00 \text{ K}$
	$\rho = A + BT + CT^2 + DT^3 + \dots$
<i>A</i>	$1.98127 \cdot 10^3$
<i>B</i>	$-6.26268 \cdot 10^{-1}$
<i>C</i>	$-1.19501 \cdot 10^{-3}$

cont

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

$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)
340.00	$1630.04 \pm 0.60$	-0.16	1974-hal/tow( $\square$ )	420.00	$1507.17 \pm 1.00$	-0.27	1974-hal/tow( $\square$ )
350.00	$1615.10 \pm 0.60$	-0.59	1974-hal/tow( $\square$ )	440.00	$1474.55 \pm 1.00$	0.19	1974-hal/tow( $\square$ )
360.00	$1601.70 \pm 0.60$	0.76	1974-hal/tow( $\square$ )	460.00	$1440.69 \pm 1.00$	0.36	1974-hal/tow( $\square$ )
370.00	$1587.12 \pm 0.60$	1.16	1974-hal/tow( $\square$ )	480.00	$1405.53 \pm 1.00$	0.20	1974-hal/tow( $\square$ )
380.00	$1569.88 \pm 0.60$	-0.85	1974-hal/tow( $\square$ )	490.00	$1387.37 \pm 1.00$	-0.11	1974-hal/tow( $\square$ )
400.00	$1538.88 \pm 1.00$	-0.68	1974-hal/tow( $\square$ )				

**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.)

cont.

**1,2,3-Trichlorotrifluorobenzene (cont.)****Table 3.** Recommended values (fit to the reliable experimental values according to the equations

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

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
340.00	$1630.20 \pm 0.81$	400.00	$1539.56 \pm 0.81$	460.00	$1440.33 \pm 1.06$
350.00	$1615.69 \pm 0.77$	410.00	$1523.62 \pm 0.82$	470.00	$1422.95 \pm 1.19$
360.00	$1600.94 \pm 0.75$	420.00	$1507.44 \pm 0.84$	480.00	$1405.33 \pm 1.36$
370.00	$1585.96 \pm 0.76$	430.00	$1491.02 \pm 0.87$	490.00	$1387.48 \pm 1.58$
380.00	$1570.73 \pm 0.77$	440.00	$1474.36 \pm 0.91$	500.00	$1369.39 \pm 1.85$
390.00	$1555.27 \pm 0.79$	450.00	$1457.46 \pm 0.97$		

**1,3,5-Trichlorotrifluorobenzene****[319-88-0]** **$C_6Cl_3F_3$** **MW = 235.42****934****Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):

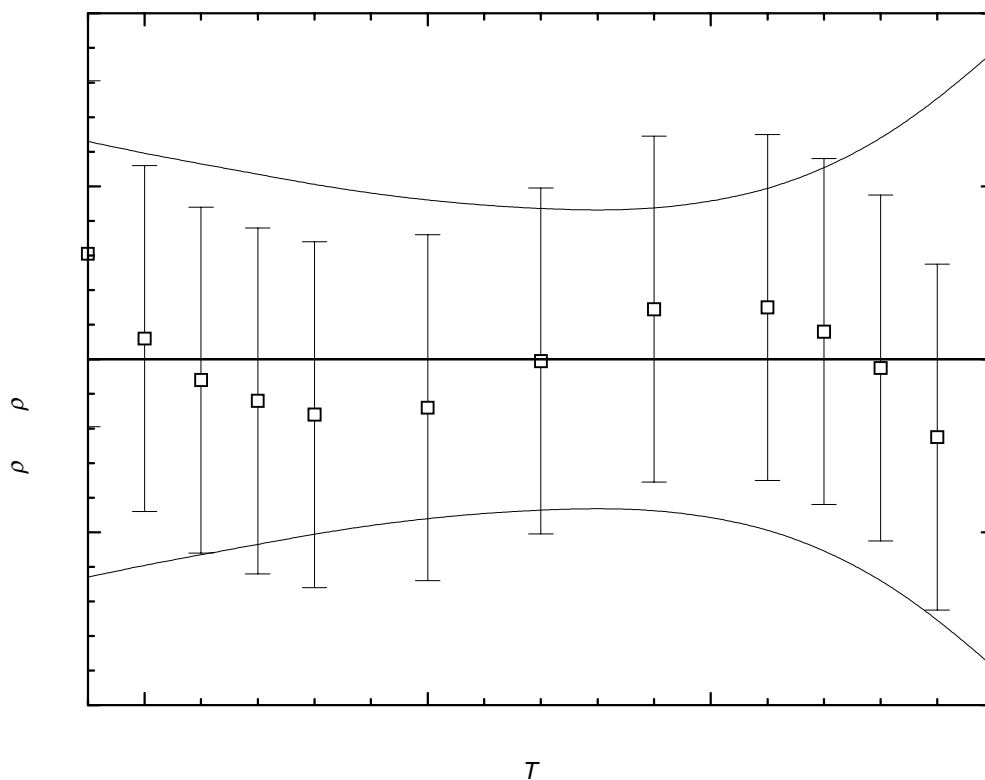
$\sigma_{c,w} = 3.4013 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 9.3147 \cdot 10^{-2}$  (combined temperature ranges, unweighted).

Coefficient	$T = 340.00 \text{ to } 490.00 \text{ K}$ $\rho = A + BT + CT^2 + DT^3 + \dots$
<i>A</i>	$1.98039 \cdot 10^3$
<i>B</i>	$-6.30818 \cdot 10^{-1}$
<i>C</i>	$-1.18063 \cdot 10^{-3}$

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

$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)
340.00	$1630.04 \pm 1.00$	0.61	1974-hal/tow(□)	420.00	$1507.17 \pm 1.00$	-0.01	1974-hal/tow(□)
350.00	$1615.10 \pm 1.00$	0.12	1974-hal/tow(□)	440.00	$1474.55 \pm 1.00$	0.29	1974-hal/tow(□)
360.00	$1600.17 \pm 1.00$	-0.12	1974-hal/tow(□)	460.00	$1440.69 \pm 1.00$	0.30	1974-hal/tow(□)
370.00	$1585.12 \pm 1.00$	-0.24	1974-hal/tow(□)	470.00	$1423.27 \pm 1.00$	0.16	1974-hal/tow(□)
380.00	$1569.88 \pm 1.00$	-0.32	1974-hal/tow(□)	480.00	$1405.53 \pm 1.00$	-0.05	1974-hal/tow(□)
400.00	$1538.88 \pm 1.00$	-0.28	1974-hal/tow(□)	490.00	$1387.37 \pm 1.00$	-0.45	1974-hal/tow(□)

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

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

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
340.00	$1629.43 \pm 1.26$	400.00	$1539.16 \pm 0.92$	460.00	$1440.39 \pm 0.98$
350.00	$1614.98 \pm 1.19$	410.00	$1523.29 \pm 0.89$	470.00	$1423.11 \pm 1.10$
360.00	$1600.29 \pm 1.13$	420.00	$1507.18 \pm 0.87$	480.00	$1405.58 \pm 1.27$
370.00	$1585.36 \pm 1.07$	430.00	$1490.84 \pm 0.86$	490.00	$1387.82 \pm 1.50$
380.00	$1570.20 \pm 1.01$	440.00	$1474.26 \pm 0.87$	500.00	$1369.82 \pm 1.78$
390.00	$1554.80 \pm 0.96$	450.00	$1457.45 \pm 0.91$		

**1-Chloro-3-(trifluoromethyl)benzene** [98-15-7]  $C_7H_4ClF_3$  MW = 180.56 935

**Table 1.** Experimental value with uncertainty.

$T$ K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ $\text{kg} \cdot \text{m}^{-3}$	Ref.
303.15	$1334.50 \pm 1.00$	1951-par/bro

**1,2-Dichloro-4-(1,1-dichloro-2,2,2-trifluoroethyl)benzene** [328-82-5]  $C_8H_3Cl_4F_3$  MW = 297.92 936

**Table 1.** Experimental value with uncertainty.

$T$ K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ $\text{kg} \cdot \text{m}^{-3}$	Ref.
298.15	$1624.40 \pm 1.00$	1951-par/bro

**1-Chloro-3-(1,1-dichloro-2,2,2-trifluoroethyl)benzene** [309-12-6]  $C_8H_4Cl_3F_3$  MW = 263.47 937

**Table 1.** Experimental value with uncertainty.

$T$ K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ $\text{kg} \cdot \text{m}^{-3}$	Ref.
298.15	$1517.30 \pm 1.00$	1951-par/bro