

## 7. Tabulated Data on Density - Nitriles

### 7.1 Saturated Nitriles

#### 7.1.1 Saturated Nitriles, C<sub>1</sub> - C<sub>7</sub>

Methanenitrile

[74-90-8]

CHN

MW = 27.03

659

**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{c,w} = 2.5993 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 1.0673 \cdot 10^{-1}$  (combined temperature ranges, unweighted).

Coefficient	T = 260.15 to 293.15 K $\rho = A + BT + CT^2 + DT^3 + \dots$
A	$1.08122 \cdot 10^3$
B	-1.34054

**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)
<i>crystal</i>				267.15	$723.00 \pm 0.60$	-0.09	1931-fre(□)
258.15	$967.0 \pm 4.0$		1951-dul/lip	269.15	$720.40 \pm 0.60$	-0.01	1931-fre(□)
<i>liquid</i>				273.15	$715.00 \pm 0.60$	-0.05	1931-fre(□)
291.15	$690.90 \pm 0.60$	-0.02	1927-bre/shi(○)	277.15	$709.60 \pm 0.60$	-0.09	1931-fre(□)
291.15	$691.30 \pm 1.00$	0.38	1927-shi(Δ)	279.15	$707.00 \pm 0.60$	-0.01	1931-fre(□)
291.15	$691.90 \pm 1.00$	0.98	1927-shi-2(×)	283.15	$701.70 \pm 0.60$	0.06	1931-fre(□)
291.15	$690.02 \pm 1.00$	-0.90	1931-coa/har(V)	288.15	$695.00 \pm 0.60$	0.06	1931-fre(□)
260.15	$732.60 \pm 0.60$	0.12	1931-fre(□)	293.15	$688.40 \pm 0.60$	0.16	1931-fre(□)
263.15	$728.50 \pm 0.60$	0.05	1931-fre(□)	293.15	$687.60 \pm 1.00$	-0.64	1932-low/hen(◆)

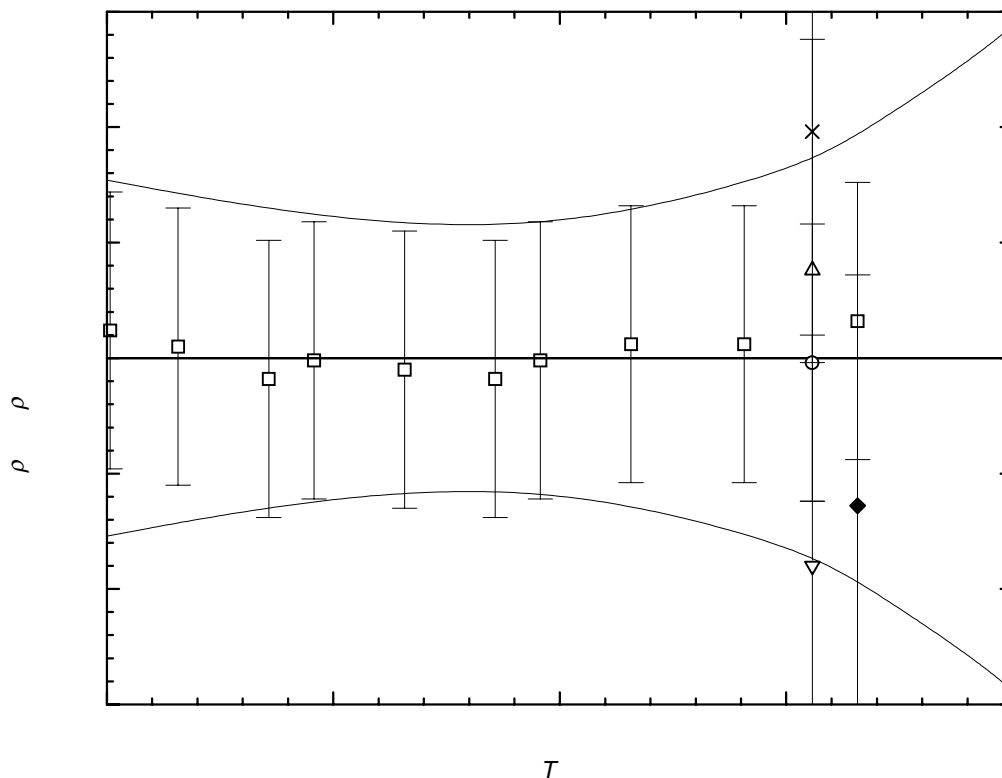
**Further references:** [1921-mey/hop, 1926-wal/mar, 1933-car, 1936-coa/tay, 1950-coa/dav].

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

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

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
260.00	$732.68 \pm 0.77$	290.00	$692.46 \pm 0.80$	300.00	$679.06 \pm 1.44$
270.00	$719.27 \pm 0.59$	293.15	$688.24 \pm 0.96$		
280.00	$705.87 \pm 0.55$	298.15	$681.54 \pm 1.29$		

cont.

**Methanenitrile** (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.)

**Ethanenitrile**

[75-05-8]

C<sub>2</sub>H<sub>3</sub>N

MW = 41.05

660

**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{c,w} = 1.3710$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 3.6823 \cdot 10^{-1}$  (combined temperature ranges, unweighted).

Coefficient	T = 233.48 to 453.15 K
	$\rho = A + BT + CT^2 + DT^3 + \dots$
A	$1.03411 \cdot 10^3$
B	$-6.34954 \cdot 10^{-1}$
C	$-7.63059 \cdot 10^{-4}$

cont.

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

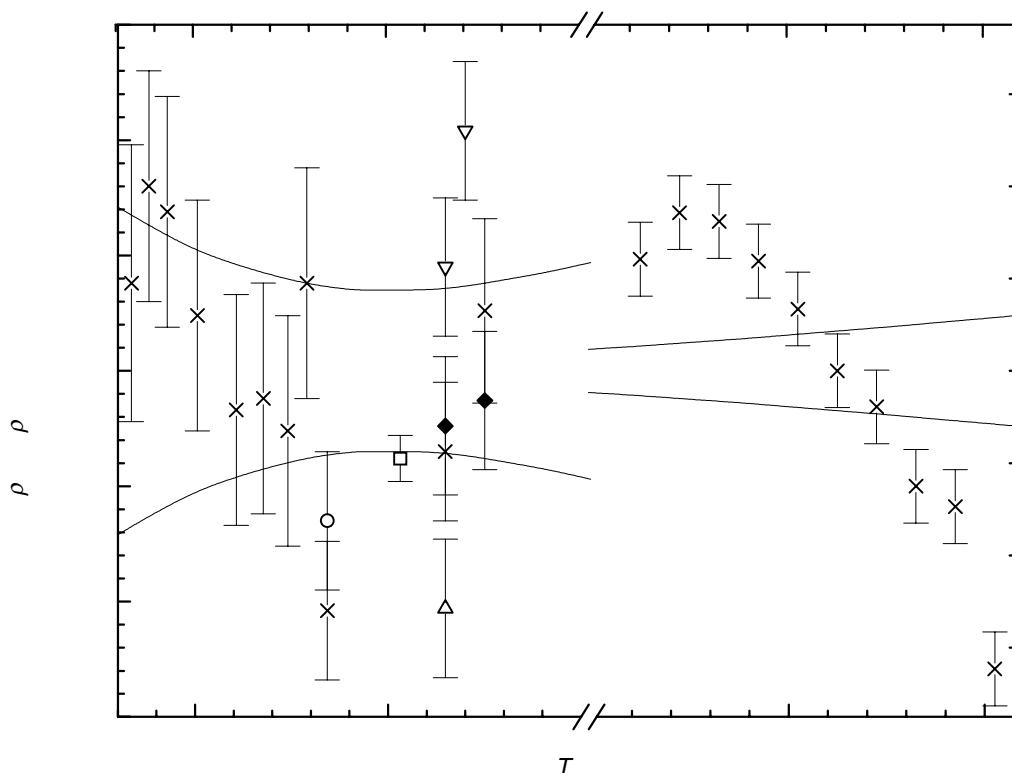
$T$ K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ kg · m <sup>-3</sup>	$\rho_{\text{exp}} - \rho_{\text{calc}}$ kg · m <sup>-3</sup>	Ref. (Symbol in Fig. 1)	$T$ K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ kg · m <sup>-3</sup>	$\rho_{\text{exp}} - \rho_{\text{calc}}$ kg · m <sup>-3</sup>	Ref. (Symbol in Fig. 1)
233.48	844.64 ± 0.60	0.38	1907-tim(×)	313.15	760.20 ± 0.30	-0.25	1989-pae/con(◆)
273.55	803.25 ± 0.65	-0.07	1907-tim <sup>1)</sup>	323.15	749.10 ± 0.30	-0.14	1989-pae/con(◆)
273.15	803.48 ± 0.60	-0.26	1910-tim <sup>1)</sup>	298.15	775.90 ± 0.30	-1.07	1991-mou/pan <sup>1)</sup>
273.15	803.48 ± 0.60	-0.26	1912-tim <sup>1)</sup>	303.15	771.70 ± 0.30	0.20	1991-mou/pan <sup>1)</sup>
237.85	840.72 ± 0.50	0.80	1912-tim-1(×)	308.15	766.20 ± 0.30	0.21	1991-mou/pan <sup>1)</sup>
242.55	835.90 ± 0.50	0.69	1912-tim-1(×)	313.15	760.90 ± 0.30	0.45	1991-mou/pan(∇)
250.20	827.72 ± 0.50	0.24	1912-tim-1(×)	318.15	755.90 ± 0.30	1.04	1991-mou/pan(∇)
260.05	817.22 ± 0.50	-0.17	1912-tim-1(×)	363.15	705.32 ± 0.80	2.42	1994-war(×)
266.95	810.11 ± 0.50	-0.12	1912-tim-1(×)	373.15	694.36 ± 0.80	3.43	1994-war(×)
273.15	803.48 ± 0.50	-0.26	1912-tim-1(×)	383.15	682.05 ± 0.80	3.24	1994-war(×)
291.35	784.15 ± 0.50	-0.19	1912-tim-1 <sup>1)</sup>	393.15	668.91 ± 0.80	2.38	1994-war(×)
303.16	771.11 ± 0.10	-0.38	1983-lop/pan(□)	403.15	655.45 ± 0.80	1.34	1994-war(×)
278.00	799.00 ± 0.50	0.38	1984-chi/twu(×)	413.15	641.53 ± 0.80	0.00	1994-war(×)
283.15	792.49 ± 0.30	-0.65	1986-dav/afa(○)	423.15	628.02 ± 0.80	-0.78	1994-war(×)
298.15	776.39 ± 0.30	-0.58	1986-dav/afa <sup>1)</sup>	433.15	613.41 ± 0.80	-2.50	1994-war(×)
283.15	792.10 ± 0.30	-1.04	1988-gar/ort(×)	443.15	599.94 ± 0.80	-2.94	1994-war(×)
293.15	781.60 ± 0.30	-0.80	1988-gar/ort <sup>1)</sup>	453.15	583.23 ± 0.80	-6.46	1994-war(×)
303.15	771.50 ± 0.30	0.00	1988-gar/ort <sup>1)</sup>	463.15	567.18 ± 0.80	-9.17	1994-war <sup>1)</sup>
313.15	760.10 ± 0.30	-0.35	1988-gar/ort(×)	298.15	776.20 ± 0.30	-0.77	1998-nik/shi <sup>1)</sup>
323.15	749.50 ± 0.40	0.26	1988-gar/ort(×)	303.15	770.80 ± 0.30	-0.70	1998-nik/shi <sup>1)</sup>
293.15	782.10 ± 0.30	-0.30	1989-pae/con <sup>1)</sup>	308.15	765.18 ± 0.30	-0.81	1998-nik/shi <sup>1)</sup>
298.15	776.60 ± 0.30	-0.37	1989-pae/con <sup>1)</sup>	313.15	759.42 ± 0.30	-1.03	1998-nik/shi(Δ)
303.15	771.00 ± 0.30	-0.50	1989-pae/con <sup>1)</sup>				

<sup>1)</sup> Not included in Fig. 1.

**Further references:** [1893-eyk, 1895-bru-1, 1902-guy/mal-1, 1906-ter, 1914-kil, 1927-von, 1930-tim/hen, 1930-zel/fre, 1932-hun/par, 1932-low/hen, 1933-mer/ver, 1935-cow/par, 1935-dar, 1935-par/cow, 1936-par, 1937-ewe, 1937-gro/sug, 1941-suh/kle, 1944-fri, 1944-fri/har-2, 1948-vog/jef, 1949-dre/mar, 1951-smi/wit, 1953-ano-6, 1954-bro/smi, 1954-bro/smi-1, 1954-tha/row, 1955-bro/smi-1, 1956-mas/sto, 1960-bro/smi, 1962-bro/smi-1, 1964-pro/ser, 1965-bla/yor, 1965-for/moo, 1967-cun/vid, 1967-mat/san-1, 1967-rus/ber, 1968-ano, 1968-vol, 1969-rus/ber, 1970-nak/shi, 1972-cur/fel, 1973-akh/mai, 1974-cla/mis, 1974-lie/mis, 1975-fra/fra, 1975-tri/ass, 1976-abs/tut, 1977-bag/kat, 1977-han, 1978-pat, 1978-siv/rao, 1979-dev/som, 1979-sub/rao, 1981-dav/ped, 1981-kor/kov, 1982-dha/nar, 1983-jan/lop, 1983-mon, 1984-ped/sal, 1985-kra/mul-1, 1985-mat/ben, 1985-nag-1, 1985-nag-2, 1985-nag-3, 1986-rit/pap, 1986-san/sha, 1987-fre, 1987-nag, 1988-fra/com, 1988-nag, 1988-nag-1, 1988-nag-4, 1988-sur/ram-1, 1991-gro/rou, 1991-mat/ber-1, 1993-hai/quo].

cont.

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

$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
230.00	847.70 ± 0.71	300.00	774.95 ± 0.35	390.00	670.42 ± 0.70
240.00	837.77 ± 0.61	310.00	763.94 ± 0.35	400.00	658.04 ± 0.77
250.00	827.68 ± 0.52	320.00	752.79 ± 0.37	410.00	645.51 ± 0.84
260.00	817.44 ± 0.46	330.00	741.48 ± 0.40	420.00	632.83 ± 0.91
270.00	807.04 ± 0.41	340.00	730.02 ± 0.43	430.00	619.99 ± 0.98
280.00	796.50 ± 0.37	350.00	718.40 ± 0.47	440.00	607.00 ± 1.06
290.00	785.80 ± 0.35	360.00	706.63 ± 0.52	450.00	593.86 ± 1.13
293.15	782.40 ± 0.35	370.00	694.71 ± 0.58	460.00	580.57 ± 1.21
298.15	776.97 ± 0.35	380.00	682.64 ± 0.64		

**Propanenitrile****[107-12-0]****C<sub>3</sub>H<sub>5</sub>N****MW = 55.08****661**

**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{c,w} = 3.0857 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 5.5830 \cdot 10^{-2}$  (combined temperature ranges, unweighted).

Coefficient	T = 273.15 to 372.30 K $\rho = A + BT + CT^2 + DT^3 + \dots$
A	$1.02463 \cdot 10^3$
B	$-6.43991 \cdot 10^{-1}$
C	$-6.29695 \cdot 10^{-4}$

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

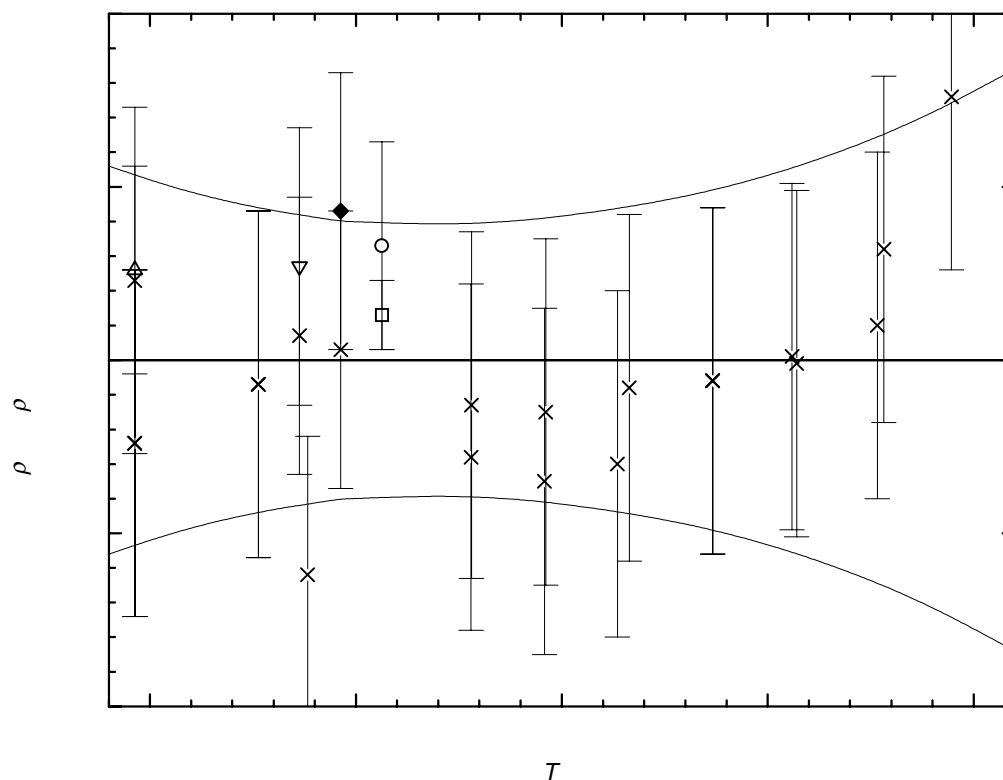
$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)
294.15	$780.10 \pm 0.40$	-0.62	1902-guy/mal-1(×)	333.20	$740.06 \pm 0.50$	-0.08	1935-dar(×)
273.15	$802.00 \pm 0.30$	0.26	1923-tim(Δ)	343.30	$729.28 \pm 0.50$	-0.06	1935-dar(×)
273.15	$801.97 \pm 0.50$	0.23	1933-mer/ver(×)	343.35	$729.22 \pm 0.50$	-0.06	1935-dar(×)
288.15	$786.71 \pm 0.50$	-0.07	1933-mer/ver(×)	352.95	$718.90 \pm 0.50$	0.01	1935-dar(×)
303.15	$771.61 \pm 0.50$	0.07	1933-mer/ver <sup>1)</sup>	353.50	$718.28 \pm 0.50$	-0.01	1935-dar(×)
303.15	$771.64 \pm 0.50$	0.10	1933-mer/ver <sup>1)</sup>	363.30	$707.66 \pm 0.50$	0.10	1935-dar(×)
303.15	$771.66 \pm 0.50$	0.12	1933-mer/ver <sup>1)</sup>	364.10	$707.00 \pm 0.50$	0.32	1935-dar(×)
273.15	$801.50 \pm 0.50$	-0.24	1934-tim/del(×)	372.30	$698.35 \pm 0.50$	0.76	1935-dar(×)
288.15	$786.71 \pm 0.50$	-0.07	1934-tim/del(×)	298.15	$777.08 \pm 0.40$	0.43	1954-tha/row(◆)
303.15	$771.94 \pm 0.50$	0.40	1934-tim/del <sup>1)</sup>	293.15	$781.80 \pm 0.40$	0.07	1958-ano-3(×)
303.15	$771.50 \pm 0.50$	-0.04	1935-dar <sup>1)</sup>	273.15	$801.50 \pm 0.50$	-0.24	1960-wri(×)
313.98	$760.08 \pm 0.50$	-0.28	1935-dar(×)	273.15	$801.50 \pm 0.50$	-0.24	1961-wri(×)
314.03	$760.17 \pm 0.50$	-0.13	1935-dar(×)	303.15	$771.87 \pm 0.30$	0.33	1966-hey/sch(○)
322.90	$750.68 \pm 0.50$	-0.35	1935-dar(×)	293.15	$782.00 \pm 0.40$	0.27	1978-pat(∇)
323.05	$750.73 \pm 0.50$	-0.15	1935-dar(×)	303.16	$771.66 \pm 0.10$	0.13	1983-lop/pan(□)
331.75	$741.39 \pm 0.50$	-0.30	1935-dar(×)	298.15	$776.68 \pm 0.40$	0.03	1993-hai/guo(×)

<sup>1)</sup> Not included in Fig. 1.

**Further references:** [1880-tho, 1884-gla, 1886-sch, 1889-gla/per, 1889-per, 1891-gla, 1893-eyk, 1895-bru-1, 1895-van, 1906-ter, 1908-wal-2, 1914-kil, 1927-fri/rod, 1927-von, 1932-low/hen, 1935-cow/par, 1941-suh/kle, 1944-fri/har-2, 1948-vog/jef, 1949-dre/mar, 1955-dun/jan, 1981-kor/kov, 1985-mat/ben, 1995-art/mun-2].

cont.

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

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
270.00	$804.85 \pm 0.56$	300.00	$774.76 \pm 0.40$	350.00	$722.10 \pm 0.53$
280.00	$794.95 \pm 0.48$	310.00	$764.48 \pm 0.39$	360.00	$711.19 \pm 0.61$
290.00	$784.92 \pm 0.43$	320.00	$754.07 \pm 0.40$	370.00	$700.15 \pm 0.71$
293.15	$781.73 \pm 0.42$	330.00	$743.54 \pm 0.43$	380.00	$688.99 \pm 0.84$
298.15	$776.65 \pm 0.40$	340.00	$732.88 \pm 0.47$		

**2-Methylpropanenitrile****[78-82-0]****C<sub>4</sub>H<sub>7</sub>N****MW = 69.11****662**

**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{c,w} = 3.0069 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 9.5134 \cdot 10^{-2}$  (combined temperature ranges, unweighted).

Coefficient	T = 273.15 to 313.16 K $\rho = A + BT + CT^2 + DT^3 + \dots$
A	$1.05704 \cdot 10^3$
B	$-9.78275 \cdot 10^{-1}$

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

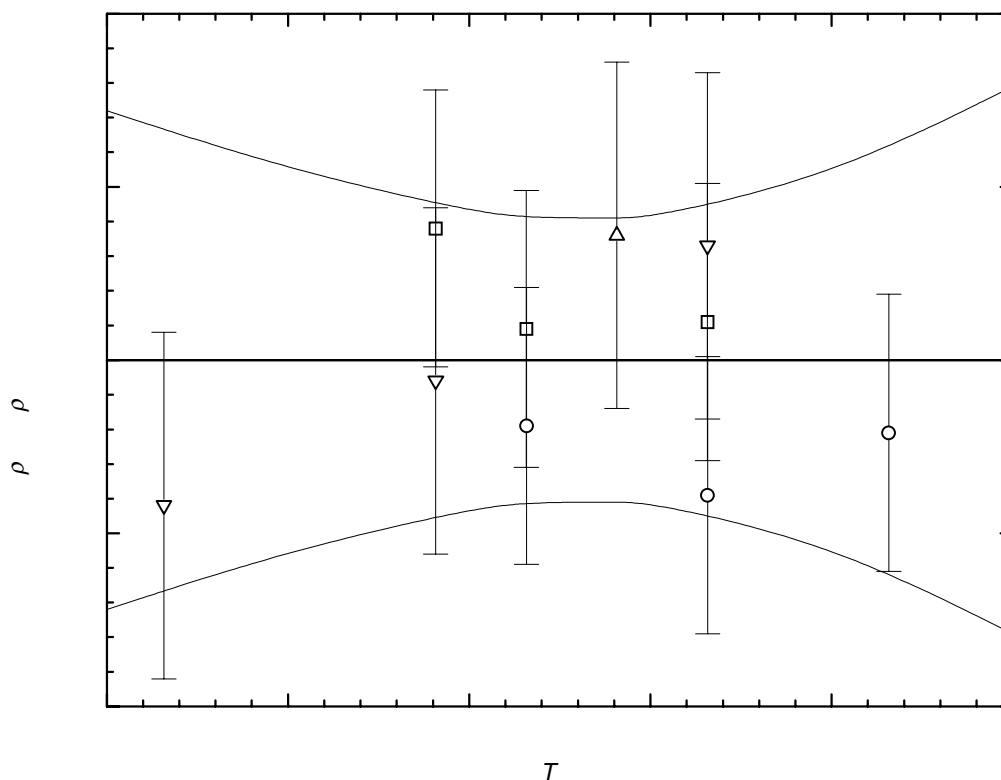
$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)
273.15	$789.40 \pm 0.50$	-0.42	1934-tim/del(∇)	303.15	$760.58 \pm 0.40$	0.11	1936-deh/bar(□)
288.15	$775.09 \pm 0.50$	-0.06	1934-tim/del(∇)	298.15	$765.72 \pm 0.50$	0.36	1947-rog-1(Δ)
303.15	$760.80 \pm 0.50$	0.33	1934-tim/del(∇)	293.16	$770.06 \pm 0.40$	-0.19	1983-lop/jan(○)
288.15	$775.53 \pm 0.40$	0.38	1936-deh/bar(□)	303.16	$760.07 \pm 0.40$	-0.39	1983-lop/jan(○)
293.15	$770.35 \pm 0.40$	0.09	1936-deh/bar(□)	313.16	$750.47 \pm 0.40$	-0.21	1983-lop/jan(○)

**Further references:** [1910-arb].

**Table 3.** Recommended values (fit to the reliable experimental values according to the equations  $\rho = A + BT + CT^2 + DT^3 + \dots$  or  $\rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)][\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3 + D(T_c - T)^4]$ ).

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
270.00	$792.90 \pm 0.72$	293.15	$770.26 \pm 0.41$	310.00	$753.77 \pm 0.53$
280.00	$783.12 \pm 0.55$	298.15	$765.36 \pm 0.41$	320.00	$743.99 \pm 0.79$
290.00	$773.34 \pm 0.43$	300.00	$763.55 \pm 0.41$		

cont.

**2-Methylpropanenitrile** (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.)

**Butanenitrile****[109-74-0]****C<sub>4</sub>H<sub>7</sub>N****MW = 69.11****663**

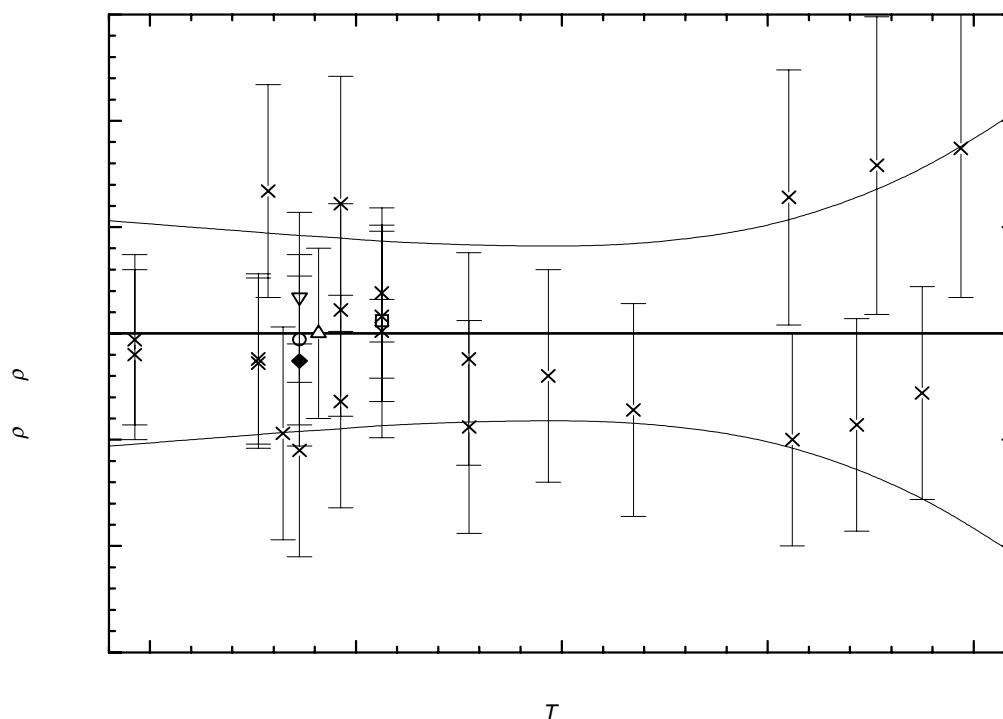
**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{c,w} = 2.8883 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 7.6544 \cdot 10^{-2}$  (combined temperature ranges, unweighted).

Coefficient	T = 273.15 to 373.45 K
	$\rho = A + BT + CT^2 + DT^3 + \dots$
A	$1.01504 \cdot 10^3$
B	$-6.04158 \cdot 10^{-1}$
C	$-5.46941 \cdot 10^{-4}$

cont.

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

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)
295.45	$788.80 \pm 0.40$	0.00	1902-guy/mal-1( $\Delta$ )	341.15	$743.83 \pm 0.50$	-1.44	1935-dar <sup>1)</sup>
288.15	$796.10 \pm 0.70$	0.56	1914-kil <sup>1)</sup>	353.00	$733.12 \pm 0.50$	-0.50	1935-dar( $\times$ )
298.15	$786.90 \pm 0.60$	0.61	1914-kil( $\times$ )	360.80	$725.43 \pm 0.50$	-0.43	1935-dar( $\times$ )
293.15	$790.38 \pm 0.50$	-0.55	1920-har/cia( $\times$ )	368.75	$717.60 \pm 0.50$	-0.28	1935-dar( $\times$ )
289.35	$795.10 \pm 0.50$	0.67	1927-von( $\times$ )	291.15	$792.30 \pm 0.50$	-0.47	1944-fri/har-2( $\times$ )
273.15	$809.17 \pm 0.40$	-0.03	1933-mer/ver( $\times$ )	313.75	$771.20 \pm 0.50$	-0.44	1944-fri/har-2( $\times$ )
288.15	$795.40 \pm 0.40$	-0.14	1933-mer/ver( $\times$ )	328.05	$753.50 \pm 0.50$	-4.48	1944-fri/har-2 <sup>1)</sup>
303.15	$781.70 \pm 0.40$	0.08	1933-mer/ver( $\times$ )	352.55	$734.70 \pm 0.60$	0.64	1944-fri/har-2( $\times$ )
273.15	$809.10 \pm 0.40$	-0.10	1934-tim/del( $\times$ )	363.25	$724.20 \pm 0.70$	0.79	1944-fri/har-2( $\times$ )
288.15	$795.42 \pm 0.40$	-0.12	1934-tim/del( $\times$ )	373.45	$714.00 \pm 0.70$	0.87	1944-fri/har-2( $\times$ )
303.15	$781.81 \pm 0.40$	0.19	1934-tim/del( $\times$ )	385.65	$702.20 \pm 0.80$	1.50	1944-fri/har-2 <sup>1)</sup>
293.15	$791.10 \pm 0.40$	0.17	1935-cow/par( $\nabla$ )	293.15	$790.90 \pm 0.40$	-0.03	1957-ano( $\circ$ )
303.15	$781.63 \pm 0.50$	0.01	1935-dar( $\times$ )	293.15	$790.80 \pm 0.40$	-0.13	1978-pat( $\blacklozenge$ )
313.70	$771.57 \pm 0.50$	-0.12	1935-dar( $\times$ )	303.16	$781.67 \pm 0.10$	0.06	1983-lop/pan( $\square$ )
323.35	$762.30 \pm 0.50$	-0.20	1935-dar( $\times$ )	298.15	$786.40 \pm 0.50$	0.11	1985-mat/ben( $\times$ )
333.70	$752.16 \pm 0.50$	-0.36	1935-dar( $\times$ )	298.15	$785.97 \pm 0.50$	-0.32	1995-art/mun-2( $\times$ )

<sup>1)</sup> Not included in Fig. 1.**Further references:** [1848-dum, 1910-tur/mer, 1944-dro/bek, 1948-vog/jef].**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.

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

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

$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
270.00	812.04 ± 0.53	300.00	784.56 ± 0.44	350.00	736.58 ± 0.50
280.00	802.99 ± 0.50	310.00	775.19 ± 0.42	360.00	726.66 ± 0.62
290.00	793.83 ± 0.47	320.00	765.70 ± 0.41	370.00	716.62 ± 0.79
293.15	790.93 ± 0.46	330.00	756.10 ± 0.41	380.00	706.48 ± 1.04
298.15	786.29 ± 0.45	340.00	746.40 ± 0.44		

**Pentanenitrile****[110-59-8]****C<sub>5</sub>H<sub>9</sub>N****MW = 83.13****664****Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):

$\sigma_{c,w} = 5.1383 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 1.0478 \cdot 10^{-1}$  (combined temperature ranges, unweighted).

Coefficient	T = 273.15 to 406.75 K $\rho = A + BT + CT^2 + DT^3 + \dots$
A	$1.04280 \cdot 10^3$
B	$-7.82595 \cdot 10^{-1}$
C	$-1.65855 \cdot 10^{-4}$

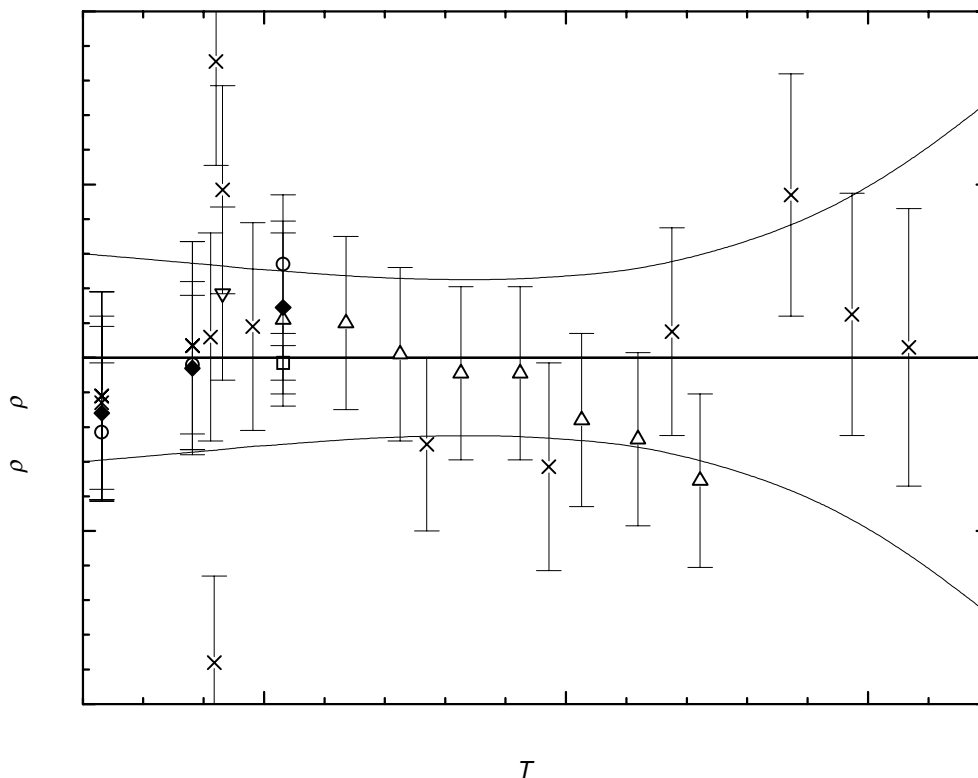
**Table 2.** Experimental values with uncertainties and deviation from calculated values.

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)
273.15	816.40 ± 0.50	-0.26	1871-lie/ros(×)	332.60	764.07 ± 0.50	-0.09	1935-dar(Δ)
291.15	801.00 ± 0.60	0.12	1884-gla(×)	342.40	755.30 ± 0.50	-0.09	1935-dar(Δ)
298.15	794.90 ± 0.60	0.18	1914-kil(×)	352.60	745.87 ± 0.50	-0.36	1935-dar(Δ)
273.15	816.44 ± 0.60	-0.22	1924-lie(×)	361.90	737.38 ± 0.50	-0.47	1935-dar(Δ)
288.15	803.59 ± 0.60	0.07	1924-lie(×)	372.20	727.83 ± 0.50	-0.71	1935-dar(Δ)
273.15	816.44 ± 0.60	-0.22	1927-van(×)	293.15	800.10 ± 0.60	0.97	1941-suh/kle(×)
288.15	803.59 ± 0.60	0.07	1927-van(×)	291.75	798.60 ± 0.50	-1.76	1944-fri/har-2(×)
292.05	801.80 ± 0.60	1.71	1927-von(×)	326.95	768.70 ± 0.50	-0.50	1944-fri/har-2(×)
273.15	816.34 ± 0.50	-0.32	1933-mer/ver(◆)	347.15	750.50 ± 0.60	-0.63	1944-fri/har-2(×)
288.15	803.46 ± 0.50	-0.06	1933-mer/ver(◆)	367.55	732.90 ± 0.60	0.15	1944-fri/har-2(×)
303.15	790.60 ± 0.50	0.29	1933-mer/ver(◆)	387.25	715.80 ± 0.70	0.94	1944-fri/har-2(×)
273.15	816.23 ± 0.40	-0.43	1934-tim/del(○)	397.35	705.90 ± 0.70	0.25	1944-fri/har-2(×)
288.15	803.48 ± 0.40	-0.04	1934-tim/del(○)	406.75	697.10 ± 0.80	0.06	1944-fri/har-2(×)
303.15	790.85 ± 0.40	0.54	1934-tim/del(○)	293.15	799.50 ± 0.50	0.37	1981-kor/kov(∇)
303.15	790.53 ± 0.50	0.22	1935-dar(Δ)	353.15	749.10 ± 0.50	3.36	1981-kor/kov <sup>1)</sup>
313.55	781.31 ± 0.50	0.20	1935-dar(Δ)	303.16	790.27 ± 0.10	-0.03	1983-lop/pan(□)
322.55	773.13 ± 0.50	0.02	1935-dar(Δ)				

<sup>1)</sup> Not included in Fig. 1.

cont.

**Further references:** [1869-gau, 1905-hen-1, 1935-cow/par, 1948-vog/jef, 1949-dre/mar].



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

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
270.00	819.40 ± 0.60	310.00	784.25 ± 0.48	370.00	730.53 ± 0.57
280.00	810.67 ± 0.57	320.00	775.38 ± 0.46	380.00	721.46 ± 0.67
290.00	801.89 ± 0.54	330.00	766.48 ± 0.45	390.00	712.36 ± 0.80
293.15	799.13 ± 0.53	340.00	757.54 ± 0.45	400.00	703.22 ± 0.98
298.15	794.72 ± 0.51	350.00	748.57 ± 0.47	410.00	694.05 ± 1.21
300.00	793.09 ± 0.51	360.00	739.57 ± 0.50	420.00	684.85 ± 1.48

**3-Methylbutanenitrile****[625-28-5]****C<sub>5</sub>H<sub>9</sub>N****MW = 83.13****665**

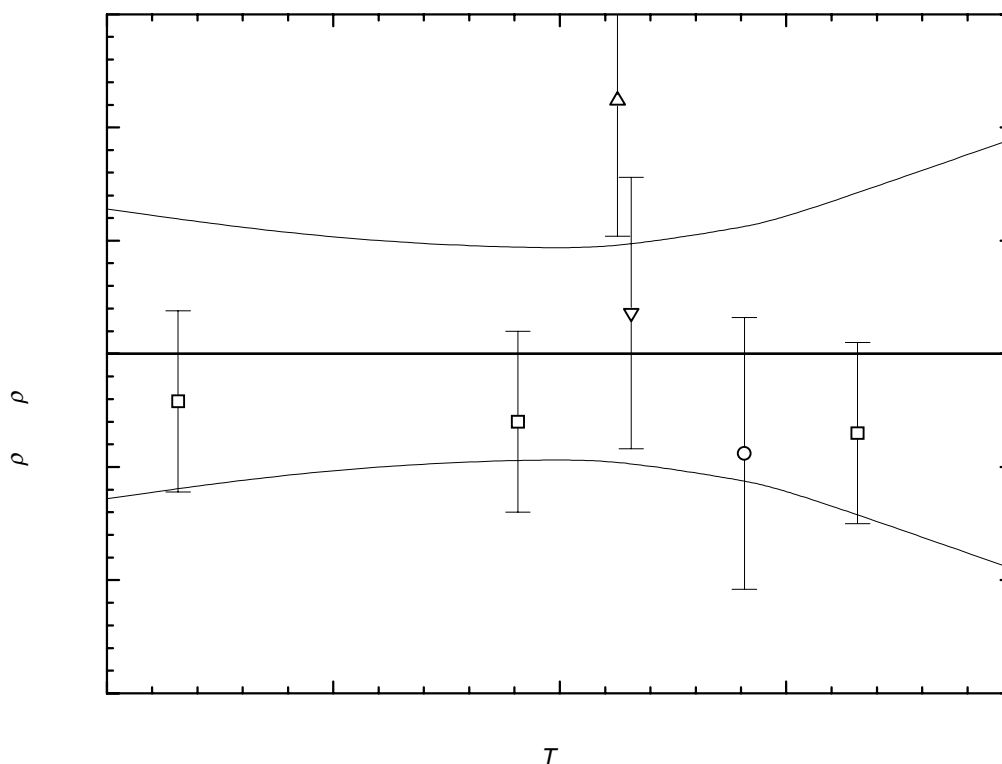
**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{c,w} = 4.2820 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 2.4071 \cdot 10^{-1}$  (combined temperature ranges, unweighted).

Coefficient	T = 273.15 to 303.15 K $\rho = A + BT + CT^2 + DT^3 + \dots$
A	$1.04437 \cdot 10^3$
B	$-8.64777 \cdot 10^{-1}$

**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	$791.04 \pm 0.60$	0.18	1920-har/cla(▽)	273.15	$807.95 \pm 0.40$	-0.21	1934-tim/del(□)
298.15	$786.10 \pm 0.60$	-0.44	1925-har/kom(○)	288.15	$794.88 \pm 0.40$	-0.30	1934-tim/del(□)
292.55	$792.50 \pm 0.60$	1.12	1927-von(Δ)	303.15	$781.86 \pm 0.40$	-0.35	1934-tim/del(□)

**Further references:** [1871-erl/hel, 1886-sch-1, 1910-arb, 1925-was].



**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.

**Table 3.** Recommended values (fit to the reliable experimental values according to the equations  $\rho = A + BT + CT^2 + DT^3 + \dots$  or  $\rho = [1 + 1.75(1 - T/T_c)^{1/3} + 0.75(1 - T/T_c)][\rho_c + A(T_c - T) + B(T_c - T)^2 + C(T_c - T)^3 + D(T_c - T)^4]$ ).

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
270.00	810.88 ± 0.64	293.15	790.86 ± 0.48	310.00	776.29 ± 0.95
280.00	802.23 ± 0.50	298.15	786.54 ± 0.56		
290.00	793.58 ± 0.46	300.00	784.94 ± 0.60		

**2,2-Dimethylpropanenitrile**

[630-18-2]

C<sub>5</sub>H<sub>9</sub>N

MW = 83.13

666

**Table 1.** Fit with estimated *B* coefficient for 5 accepted points. Deviation  $\sigma_w = 0.440$ .

Coefficient	$\rho = A + BT$
<i>A</i>	1040.17
<i>B</i>	-0.950

**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.
298.15	758.5 ± 1.0	1.62	1947-rog-1	328.15	731.0 ± 2.0	2.57	1965-kri/man <sup>1)</sup>
293.15	761.8 ± 0.4	0.13	1982-dig/jad	293.15	761.7 ± 0.5	0.02	1983-lop/jan
298.15	760.0 ± 2.0	3.07	1965-kri/man <sup>1)</sup>	303.16	752.0 ± 0.5	-0.17	1983-lop/jan
313.15	745.0 ± 2.0	2.32	1965-kri/man <sup>1)</sup>	313.16	742.2 ± 0.5	-0.47	1983-lop/jan

<sup>1)</sup> Not included in calculation of recommended value.

**Table 3.** Recommended values.

$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$
290.00	764.7 ± 1.1
293.15	761.7 ± 0.8
298.15	756.9 ± 0.6
310.00	745.7 ± 1.2
320.00	736.2 ± 2.1

**2-Methylbutanenitrile**

[18936-17-9]

C<sub>5</sub>H<sub>9</sub>N

MW = 83.13

667

**Table 1.** Fit with estimated *B* coefficient for 5 accepted points. Deviation  $\sigma_w = 0.324$ .

Coefficient	$\rho = A + BT$
<i>A</i>	1056.52
<i>B</i>	-0.920

cont.

**2-Methylbutanenitrile** (cont.)**Table 2.** Experimental values with uncertainties and deviation from calculated values.

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref.	$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref.
293.15	786.0 ± 1.0	-0.82	1935-ken/phi	288.15	791.3 ± 0.4	-0.16	1936-deh/bar
273.15	806.3 ± 1.0	1.08	1954-art/pra	293.15	786.8 ± 0.4	-0.05	1936-deh/bar
296.15	773.9 ± 3.0	-10.16	1956-wal/hor <sup>1)</sup>	303.15	777.8 ± 0.4	0.16	1936-deh/bar

<sup>1)</sup> Not included in calculation of recommended value.**Table 3.** Recommended values.

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$
270.00	808.1 ± 2.4
280.00	798.9 ± 1.5
290.00	789.7 ± 0.7
293.15	786.8 ± 0.6
298.15	782.2 ± 0.7
310.00	771.3 ± 1.7

**4-Methylpentanenitrile**

[542-54-1]

C<sub>6</sub>H<sub>11</sub>N

MW = 97.16

668

**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{\text{c,w}} = 9.1396 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{\text{c,uw}} = 2.9262 \cdot 10^{-1}$  (combined temperature ranges, unweighted).

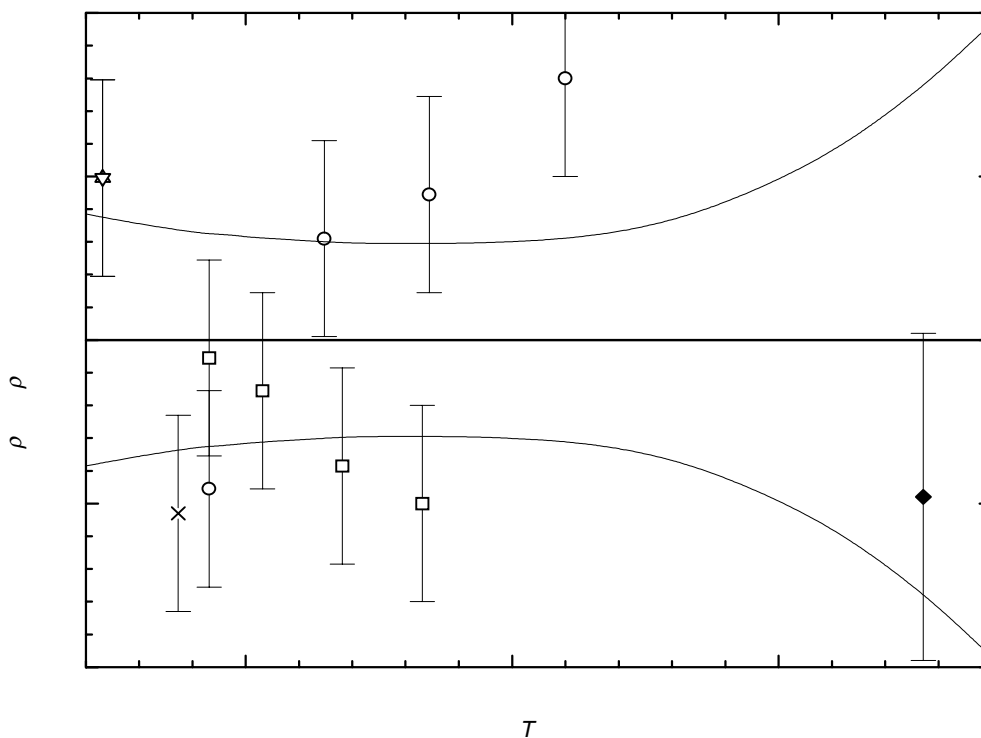
Coefficient	T = 273.15 to 427.15 K $\rho = A + BT + CT^2 + DT^3 + \dots$
A	$9.96924 \cdot 10^2$
B	$-5.11853 \cdot 10^{-1}$
C	$-5.00003 \cdot 10^{-4}$

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

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)
427.15	686.10 ± 1.00	-0.96	1886-sch(◆)	293.15	803.00 ± 0.60	-0.91	1948-vog/jef(○)
287.35	807.50 ± 0.60	-1.06	1893-eyk(×)	314.75	786.90 ± 0.60	0.62	1948-vog/jef(○)
293.15	803.80 ± 0.60	-0.11	1910-tur/mer(□)	334.45	770.70 ± 0.60	0.89	1948-vog/jef(○)
303.15	795.50 ± 0.60	-0.31	1910-tur/mer(□)	359.95	749.50 ± 0.60	1.60	1948-vog/jef(○)
318.15	782.70 ± 0.60	-0.77	1910-tur/mer(□)	273.15	820.80 ± 0.60	0.99	1960-wri(Δ)
333.15	769.90 ± 0.60	-1.00	1910-tur/mer(□)	273.15	820.80 ± 0.60	0.99	1961-wri(▽)

**Further references:** [1895-bru-1, 1927-fri/rod, 1947-rog-1].

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

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
270.00	822.27 ± 0.77	320.00	781.93 ± 0.59	390.00	721.25 ± 0.84
280.00	814.40 ± 0.71	330.00	773.56 ± 0.59	400.00	712.18 ± 0.98
290.00	806.44 ± 0.66	340.00	765.09 ± 0.59	410.00	703.01 ± 1.15
293.15	803.91 ± 0.65	350.00	756.52 ± 0.60	420.00	693.74 ± 1.37
298.15	799.87 ± 0.64	360.00	747.86 ± 0.62	430.00	684.38 ± 1.63
300.00	798.37 ± 0.63	370.00	739.09 ± 0.66	440.00	674.91 ± 1.94
310.00	790.20 ± 0.61	380.00	730.22 ± 0.73		

## 2-Ethylbutanenitrile

[617-80-1]

C<sub>6</sub>H<sub>11</sub>N

MW = 97.16

669

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

$\frac{T}{K}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref.
298.15	811.0 ± 2.0	1931-lev/mar-5

**Hexanenitrile****[628-73-9]****C<sub>6</sub>H<sub>11</sub>N****MW = 97.16****670**

**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{c,w} = 4.4252 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{c,uw} = 1.1144 \cdot 10^{-1}$  (combined temperature ranges, unweighted).

Coefficient	T = 273.15 to 429.85 K $\rho = A + BT + CT^2 + DT^3 + \dots$
A	$1.04200 \cdot 10^3$
B	$-7.82421 \cdot 10^{-1}$
C	$-8.73132 \cdot 10^{-5}$

**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	$805.90 \pm 0.60$	0.77	1924-rup/gle(×)	361.00	$748.05 \pm 0.50$	-0.12	1935-dar(∇)
273.15	$821.55 \pm 0.40$	-0.22	1929-sim(○)	370.30	$740.03 \pm 0.50$	-0.27	1935-dar(∇)
288.15	$809.37 \pm 0.40$	0.08	1929-sim(○)	290.05	$811.10 \pm 0.50$	3.39	1944-fri/har-2 <sup>1)</sup>
303.15	$797.08 \pm 0.40$	0.30	1929-sim(○)	330.85	$776.10 \pm 0.50$	2.52	1944-fri/har-2 <sup>1)</sup>
273.15	$821.69 \pm 0.40$	-0.08	1933-mer/ver(Δ)	347.05	$758.20 \pm 0.60$	-1.74	1944-fri/har-2(×)
288.15	$809.40 \pm 0.40$	0.11	1933-mer/ver(Δ)	381.65	$731.90 \pm 0.60$	1.23	1944-fri/har-2(×)
303.15	$797.11 \pm 0.40$	0.33	1933-mer/ver(Δ)	401.15	$714.80 \pm 0.70$	0.72	1944-fri/har-2(×)
303.15	$797.02 \pm 0.50$	0.24	1935-dar(∇)	421.15	$696.90 \pm 0.70$	-0.10	1944-fri/har-2(×)
312.45	$788.71 \pm 0.50$	-0.30	1935-dar(∇)	429.85	$689.20 \pm 0.80$	-0.34	1944-fri/har-2(×)
323.05	$780.34 \pm 0.50$	0.21	1935-dar(∇)	293.15	$805.18 \pm 0.40$	0.05	1949-dre/mar(□)
333.10	$771.66 \pm 0.50$	-0.03	1935-dar(∇)	298.15	$801.04 \pm 0.40$	0.08	1949-dre/mar(□)
342.35	$763.74 \pm 0.50$	-0.16	1935-dar(∇)	273.15	$821.50 \pm 0.50$	-0.27	1960-wri(◆)
352.55	$755.08 \pm 0.50$	-0.22	1935-dar(∇)	273.15	$821.50 \pm 0.50$	-0.27	1961-wri(×)

<sup>1)</sup> Not included in Fig. 1.

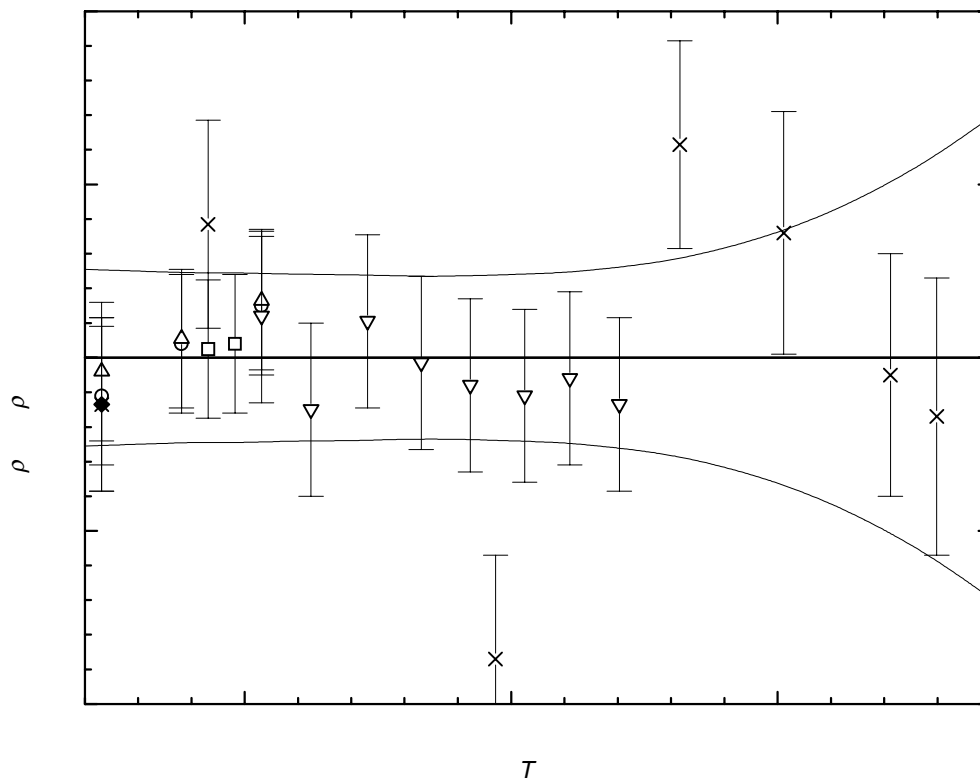
**Further references:** [1884-gla, 1895-bru-1, 1902-guy/mal-1, 1905-hen-1, 1917-jae, 1944-dro/bek, 1948-vog/jef].

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

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

$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
270.00	$824.38 \pm 0.51$	320.00	$782.68 \pm 0.48$	390.00	$723.57 \pm 0.63$
280.00	$816.08 \pm 0.50$	330.00	$774.29 \pm 0.47$	400.00	$715.06 \pm 0.72$
290.00	$807.75 \pm 0.49$	340.00	$765.88 \pm 0.47$	410.00	$706.53 \pm 0.84$
293.15	$805.13 \pm 0.49$	350.00	$757.46 \pm 0.48$	420.00	$697.98 \pm 0.99$
298.15	$800.96 \pm 0.49$	360.00	$749.01 \pm 0.49$	430.00	$689.41 \pm 1.17$
300.00	$799.41 \pm 0.49$	370.00	$740.55 \pm 0.52$	440.00	$680.83 \pm 1.39$
310.00	$791.06 \pm 0.48$	380.00	$732.07 \pm 0.56$		

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.)

## 2-Methylpentanenitrile

[6339-13-5]

C<sub>6</sub>H<sub>11</sub>N

MW = 97.16

671

**Table 1.** Fit with estimated *B* coefficient for 4 accepted points. Deviation  $\sigma_w = 0.461$ .

Coefficient	$\rho = A + BT$
<i>A</i>	1045.43
<i>B</i>	-0.860

**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.
273.60	827.2 ± 3.0	17.07	1908-har/sik <sup>1)</sup>	288.15	797.5 ± 0.4	-0.17	1936-deh/bar
292.65	807.7 ± 3.0	13.95	1909-mar/nol <sup>1)</sup>	293.15	793.2 ± 0.4	-0.12	1936-deh/bar
298.15	791.0 ± 1.0	1.98	1929-lev/mik	303.15	784.7 ± 0.4	-0.03	1936-deh/bar

<sup>1)</sup> Not included in calculation of linear coefficients.

cont.

**2-Methylpentanenitrile** (cont.)**Table 3.** Recommended values.

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$
280.00	804.6 ± 1.6
290.00	796.0 ± 0.8
293.15	793.3 ± 0.6
298.15	789.0 ± 0.6
310.00	778.8 ± 1.6

**d-3-Methylpentanenitrile**

[500044-89-3]

C<sub>6</sub>H<sub>11</sub>N

MW = 97.16

672

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

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref.
298.15	811.0 ± 2.0	1931-lev/mar-5

**Heptanenitrile**

[629-08-3]

C<sub>7</sub>H<sub>13</sub>N

MW = 111.19

673

**Table 1.** Coefficients of the polynomial expansion equation. Standard deviations (see introduction):  $\sigma_{\text{c,w}} = 6.0708 \cdot 10^{-1}$  (combined temperature ranges, weighted),  $\sigma_{\text{c,uw}} = 1.9670 \cdot 10^{-1}$  (combined temperature ranges, unweighted).

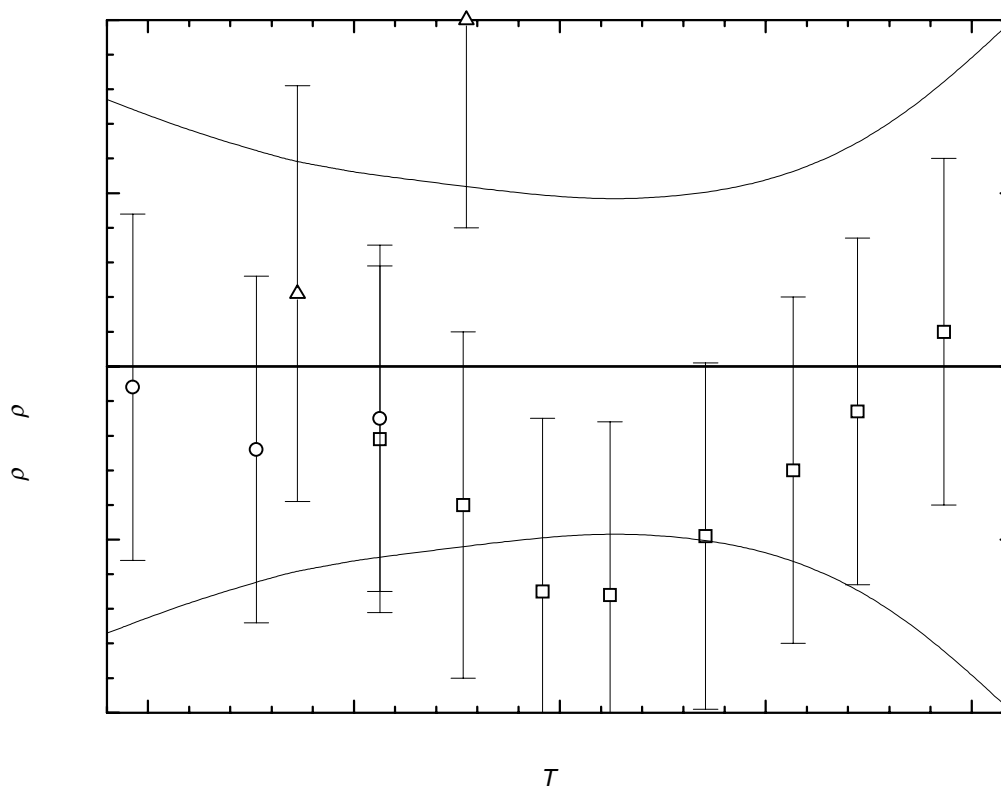
Coefficient	$T = 273.15 \text{ to } 371.65 \text{ K}$ $\rho = A + BT + CT^2 + DT^3 + \dots$
A	$9.96729 \cdot 10^2$
B	$-4.90907 \cdot 10^{-1}$
C	$-5.00682 \cdot 10^{-4}$

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

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)	$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref. (Symbol in Fig. 1)
273.15	825.22 ± 0.50	-0.06	1933-mer/ver(○)	353.35	760.45 ± 0.50	-0.30	1935-dar(□)
288.15	813.46 ± 0.50	-0.24	1933-mer/ver(○)	361.15	754.00 ± 0.50	-0.13	1935-dar(□)
303.15	801.75 ± 0.50	-0.15	1933-mer/ver(○)	371.65	745.23 ± 0.50	0.10	1935-dar(□)
303.15	801.69 ± 0.50	-0.21	1935-dar(□)	293.15	810.00 ± 0.60	0.21	1948-vog/jef(Δ)
313.27	793.41 ± 0.50	-0.40	1935-dar(□)	313.65	794.50 ± 0.60	1.00	1948-vog/jef(Δ)
322.90	785.36 ± 0.50	-0.65	1935-dar(□)	333.15	779.60 ± 0.60	1.99	1948-vog/jef(Δ)
331.10	778.64 ± 0.50	-0.66	1935-dar(□)	358.15	759.70 ± 0.60	3.01	1948-vog/jef <sup>1)</sup>
342.70	769.20 ± 0.50	-0.49	1935-dar(□)				

<sup>1)</sup> Not included in Fig. 1.**Further references:** [1877-meh].

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

$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{T}{\text{K}}$	$\frac{\rho \pm \sigma_{\text{fit}}}{\text{kg} \cdot \text{m}^{-3}}$
270.00	$827.68 \pm 0.77$	300.00	$804.40 \pm 0.56$	350.00	$763.58 \pm 0.53$
280.00	$820.02 \pm 0.68$	310.00	$796.43 \pm 0.53$	360.00	$755.11 \pm 0.62$
290.00	$812.26 \pm 0.61$	320.00	$788.37 \pm 0.50$	370.00	$746.55 \pm 0.78$
293.15	$809.79 \pm 0.59$	330.00	$780.21 \pm 0.48$	380.00	$737.89 \pm 1.00$
298.15	$805.86 \pm 0.57$	340.00	$771.94 \pm 0.49$		

**2-Methylhexanenitrile** [20654-42-6] C<sub>7</sub>H<sub>13</sub>N MW = 111.19 674

**Table 1.** Fit with estimated  $B$  coefficient for 3 accepted points. Deviation  $\sigma_w = 0.349$ .

Coefficient	$\rho = A + BT$
$A$	1040.27
$B$	-0.820

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

$T$ K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ kg·m <sup>-3</sup>	$\rho_{\text{exp}} - \rho_{\text{calc}}$ kg·m <sup>-3</sup>	Ref.
298.15	797.0 ± 1.0	1.21	1929-lev/mik
288.15	803.8 ± 0.4	-0.17	1935-deh/bar
303.15	791.7 ± 0.4	-0.02	1935-deh/bar

**Table 3.** Recommended values.

$T$ K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ kg·m <sup>-3</sup>
280.00	810.7 ± 1.0
290.00	802.5 ± 0.7
293.15	799.9 ± 0.7
298.15	795.8 ± 0.7
310.00	786.1 ± 1.0

**2-Ethyl-2-methylbutanenitrile** [21864-76-6] C<sub>7</sub>H<sub>13</sub>N MW = 111.19 675

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

$T$ K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ kg·m <sup>-3</sup>	Ref.
298.15	803.4 ± 2.0	1960-pro/bur

**3-Methylhexanenitrile** [53783-89-4] C<sub>7</sub>H<sub>13</sub>N MW = 111.19 676

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

$T$ K	$\rho_{\text{exp}} \pm 2\sigma_{\text{est}}$ kg·m <sup>-3</sup>	Ref.
293.15	810.9 ± 0.7	1924-dew/wec

**4-Methylhexanenitrile****[69248-32-4]****C<sub>7</sub>H<sub>13</sub>N****MW = 111.19****677****Table 1.** Fit with estimated *B* coefficient for 2 accepted points. Deviation  $\sigma_w = 0.268$ .

Coefficient	$\rho = A + BT$
<i>A</i>	1048.75
<i>B</i>	-0.800

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

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	$\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref.
293.15	814.1 ± 0.7	-0.13	1924-dew/wec
299.15	810.0 ± 1.5	0.57	1931-lev/mar-5

**Table 3.** Recommended values.

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$
290.00	816.7 ± 1.1
293.15	814.2 ± 1.0
298.15	810.2 ± 1.1

***l*-3-Methylhexanenitrile****[500044-90-6]****C<sub>7</sub>H<sub>13</sub>N****MW = 111.19****678****Table 1.** Experimental value with uncertainty.

$\frac{T}{\text{K}}$	$\frac{\rho_{\text{exp}} \pm 2\sigma_{\text{est}}}{\text{kg} \cdot \text{m}^{-3}}$	Ref.
299.15	810.0 ± 2.0	1931-lev/mar-5