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Orthobaric densities and molar volumes of liquids

Part 1A

C_1 to C_{18} alkanes

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ORTHOBARIC DENSITIES AND MOLAR VOLUMES OF LIQUIDS

PART 1A: C₁ TO C₁₈ ALKANES

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ORTHOBARIC DENSITIES AND MOLAR VOLUMES OF LIQUIDS

PART 1A: C₁ TO C₁₈ ALKANES

1. INTRODUCTION

This Data Item presents orthobaric liquid densities and molar volumes of the C₁ to C₁₈ alkanes listed in Table 1 (pages 2 and 3), with alternative names, if any.

The values of density and molar volume given in the Tables have been obtained by evaluating, for each compound, an equation of the form

$$\ln(d/d_c) = -\ln(V/V_c) = a_1q + a_2q^2 + a_3q^3 + a_4q^4. \quad (1)$$

Equation (1) was fitted to the experimental data that had been selected and weighted in accordance with a critical assessment of all the data (see Sections A.2 and A.3). Table 2 gives the molecular weight, critical temperature, critical density and the coefficients a_1 , a_2 , a_3 and a_4 for each compound to be used in Equation (1).

Tables 3(D) to 11(D) present values of density in kg/m³ from the freezing point, T_f , to the critical point at intervals of 10°C. Tables 3(V) to 11(V) present molar volumes in cm³/mol over the same temperature range at intervals of 10 K.

The number of decimal places in each value of density and molar volume in the Tables indicates the reliability of the experimental data on which the values are based. Values with two decimal places are considered to have an uncertainty between 0.01 and 0.1 per cent. Values with one decimal place are considered to have an uncertainty between 0.1 and 1.0 per cent and values with no decimal places an uncertainty between 1 and 10 per cent.

The sources of experimental data for each compound, on which the tabulated values are based, and the calculation procedure are detailed in Appendix A which also contains a summary of the critical constants of all the compounds.

2. NOTATION

a_1, a_2, a_3, a_4	non-dimensional constants for each compound in Equation (1)	
d	density	kg/m ³
p	saturation pressure	kPa
q	$(1-T_r)^{1/3}$	
M.W.	molecular weight	
R	gas constant, 8.3143	J/mol K
T	temperature on the International Practical Temperature Scale 1968, IPTS 68, (273.15 + °C)	K
V	molar volume	cm ³ /mol
Z	compression factor ($pV/1000RT$)	
suffices		
c	denotes value at critical point	
f	denotes value at freezing point	
r	denotes reduced quantity, e.g. $T_r = T/T_c$	

TABLE 1

LIST of COMPOUNDS

The Empirical Formula, Name, Alternative Name, if any, and location of the Tables giving the Saturated Liquid Density, d, and the Saturated Liquid Molar Volume, V, for each compound considered in this Data Item are as follows.

No.	Emp. Form.	Name	Alternative Names	Table Pages d V
C ₁ to C ₃ ALKANES				
1	CH ₄	Methane		6 15
2	C ₂ H ₆	Ethane		6 15
3	C ₃ H ₈	Propane		6 15
C ₄ ALKANES				
4	C ₄ H ₁₀	Butane	n-Butane	6 15
5		2-Methylpropane	Isobutane	6 15
C ₅ ALKANES				
6	C ₅ H ₁₂	Pentane	n-Pentane	6 15
7		2-Methylbutane	Isopentane	6 15
8		2,2-Dimethylpropane	Neopentane	6 15
C ₆ ALKANES				
9	C ₆ H ₁₄	Hexane	n-Hexane	7 16
10		2-Methylpentane	Isohexane	7 16
11		3-Methylpentane		7 16
12		2,2-Dimethylbutane	Neohexane	7 16
13		2,3-Dimethylbutane	Diisopropyl	7 16
C ₇ ALKANES				
14	C ₇ H ₁₆	Heptane	n-Heptane	8 17
15		2-Methylhexane		8 17
16		3-Methylhexane		8 17
17		3-Ethylpentane	Triethylmethane	8 17
18		2,2-Dimethylpentane		9 18
19		2,3-Dimethylpentane		9 18
20		2,4-Dimethylpentane		9 18
21		3,3-Dimethylpentane		9 18
22		2,2,3-Trimethylbutane	Triptane	9 18
C ₈ ALKANES				
23	C ₈ H ₁₈	Octane	n-Octane	10 19
24		2-Methylheptane		10 19
25		3-Methylheptane		10 19
26		4-Methylheptane		10 19
27		3-Ethylhexane		10 19
28		2,2-Dimethylhexane		11 20
29		2,3-Dimethylhexane		11 20
30		2,4-Dimethylhexane		11 20
31		2,5-Dimethylhexane		11 20
32		3,3-Dimethylhexane		11 20
33		3,4-Dimethylhexane		11 20
34		2-Methyl-3-ethylpentane		12 21
35		3-Methyl-3-ethylpentane		12 21
36		2,2,3-Trimethylpentane		12 21
37		2,2,4-Trimethylpentane	Isooctane	12 21
38		2,3,3-Trimethylpentane		12 21
39		2,3,4-Trimethylpentane		12 21
40		2,2,3,3-Tetramethylbutane	Hexamethylethane	12 21

TABLE 1 continued
LIST of COMPOUNDS continued

No.	Emp. Form.	Name	Alternative Names	Table Pages d V
		C ₉ to C ₁₈ ALKANES		
41	C ₉ H ₂₀	Nonane	n-Nonane	13 22
42	C ₁₀ H ₂₂	Decane	n-Decane	13 22
43	C ₁₁ H ₂₄	Undecane	n-Undecane	13 22
44	C ₁₂ H ₂₆	Dodecane	n-Dodecane	13 22
45	C ₁₃ H ₂₈	Tridecane	n-Tridecane	13 22
46	C ₁₄ H ₃₀	Tetradecane	n-Tetradecane	14 23
47	C ₁₅ H ₃₂	Pentadecane	n-Pentadecane	14 23
48	C ₁₆ H ₃₄	Hexadecane	n-Hexadecane	14 23
49	C ₁₇ H ₃₆	Heptadecane	n-Heptadecane	14 23
50	C ₁₈ H ₃₈	Octadecane	n-Octadecane	14 23

TABLE 2
CONSTANTS in EQUATION (1)

This Table lists the constants for each compound that, when used in Equation (1) give the Saturated Liquid Density, d , and the Saturated Liquid Molar Volume, V , given on pages 6 to 14 and pages 15 to 23 respectively.

No.	Name	T_c K	d_c kg/m ³	a_1	a_2	a_3	a_4
C₁ to C₃ ALKANES							
1	Methane	190.56	162.66	1.50636	-0.26215	-0.18911	0.17951
2	Ethane	305.33	206.9	1.56860	-0.27416	-0.33237	0.32404
3	Propane	369.85	220.3	1.62195	-0.31345	-0.37486	0.37979
C₄ ALKANES							
4	Butane	425.25	229	1.64250	-0.32433	-0.38920	0.39579
5	2-Methylpropane	407.85	227	1.63164	-0.31738	-0.38086	0.38560
C₅ ALKANES							
6	Pentane	469.80	232	1.68461	-0.35127	-0.42153	0.43531
7	2-Methylbutane	460.45	235	1.64647	-0.32688	-0.39226	0.39953
8	2,2-Dimethylpropane	433.75	234	1.60355	-0.29941	-0.35929	0.35923
C₆ ALKANES							
9	Hexane	507.90	234	1.71086	-0.36808	-0.44170	0.45997
10	2-Methylpentane	497.85	236	1.68367	-0.35068	-0.42081	0.43444
11	3-Methylpentane	504.45	235	1.72772	-0.37884	-0.45461	0.47576
12	2,2-Dimethylbutane	489.35	248	1.54862	-0.26425	-0.31709	0.30765
13	2,3-Dimethylbutane	500.25	248	1.57717	-0.28253	-0.33903	0.33447
C₇ ALKANES							
14	Heptane	540.15	236	1.72312	-0.37591	-0.45110	0.47146
15	2-Methylhexane	530.35	241	1.66321	-0.33757	-0.40509	0.41521
16	3-Methylhexane	535.25	241	1.68782	-0.35332	-0.42399	0.43832
17	3-Ethylpentane	540.65	241	1.72096	-0.37453	-0.44944	0.46943
18	2,2-Dimethylpentane	520.55	247	1.59577	-0.29443	-0.35331	0.35192
19	2,3-Dimethylpentane	537.35	246	1.65949	-0.33519	-0.40223	0.41173
20	2,4-Dimethylpentane	519.75	246	1.60358	-0.29943	-0.35932	0.35926
21	3,3-Dimethylpentane	536.35	247	1.64324	-0.32480	-0.38976	0.39648
22	2,2,3-Trimethylbutane	531.15	251	1.59677	-0.29506	-0.35407	0.35285
C₈ ALKANES							
23	Octane	568.95	237	1.73439	-0.38312	-0.45975	0.48204
24	2-Methylheptane	559.65	242	1.67581	-0.34564	-0.41477	0.42704
25	3-Methylheptane	563.65	242	1.69910	-0.36055	-0.43266	0.44891
26	4-Methylheptane	561.75	242	1.69763	-0.35960	-0.43152	0.44753
27	3-Ethylhexane	565.45	242	1.72602	-0.37777	-0.45332	0.47418
28	2,2-Dimethylhexane	549.85	247	1.62695	-0.31438	-0.37725	0.38119
29	2,3-Dimethylhexane	563.45	246	1.67964	-0.34810	-0.41772	0.43066
30	2,4-Dimethylhexane	553.55	246	1.65107	-0.32981	-0.39577	0.40383
31	2,5-Dimethylhexane	550.05	246	1.63070	-0.31678	-0.38014	0.38472
32	3,3-Dimethylhexane	562.05	247	1.66259	-0.33719	-0.40462	0.41465
33	3,4-Dimethylhexane	568.85	246	1.69710	-0.35926	-0.43111	0.44703
34	2-Methyl-3-ethylpentane	567.05	246	1.70057	-0.36149	-0.43379	0.45029
35	3-Methyl-3-ethylpentane	576.55	247	1.70522	-0.36445	-0.43734	0.45465
36	2,2,3-Trimethylpentane	563.55	251	1.64034	-0.32294	-0.38753	0.39375
37	2,2,4-Trimethylpentane	543.85	250	1.59153	-0.29168	-0.35002	0.34790
38	2,3,3-Trimethylpentane	573.55	251	1.66268	-0.33725	-0.40470	0.41474
39	2,3,4-Trimethylpentane	566.45	250	1.65751	-0.33393	-0.40072	0.40987
40	2,2,3,3-Tetramethylbutane	568.15	265	1.51711	-0.24409	-0.29290	0.27808

TABLE 2 continued
CONSTANTS in EQUATION (1) continued

No.	Name	T_c K	d_c kg/m ³	a_1	a_2	a_3	a_4
C ₉ to C ₁₈ ALKANES							
41	Nonane	594.65	238	1.74086	-0.38726	-0.46471	0.48810
42	Decane	617.65	239	1.74387	-0.38919	-0.46703	0.49094
43	Undecane	638.85	240	1.75516	-0.42605	-0.49926	0.54958
44	Dodecane	658.65	240	1.77472	-0.44678	-0.53613	0.61130
45	Tridecane	676.15	240	1.78888	-0.46903	-0.56283	0.65600
46	Tetradecane	693.15	241	1.77745	-0.45107	-0.54128	0.61990
47	Pentadecane	708.15	241	1.78152	-0.45746	-0.54895	0.63274
48	Hexadecane	722.15	241	1.79165	-0.47338	-0.56806	0.66471
49	Heptadecane	735.15	241	1.79743	-0.48246	-0.57895	0.68293
50	Octadecane	748.15	241	1.80098	-0.48804	-0.58565	0.69414

SATURATED LIQUID DENSITY of C₁ to C₅ ALKANES

1	CH_4	Methane	
2	C_2H_6	Ethane	
3	C_3H_8	Propane	
4	C_4H_{10}	Butane	n-Butane
5		2-Methylpropane	Isobutane
6	C_5H_{12}	Pentane	n-Pentane
7		2-Methylbutane	Isopentane
8		2,2-Dimethylpropane	Neopentane

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TABLE 4(D)
SATURATED LIQUID DENSITY of C₆ ALKANES

Units: kg/m³ v. deg.C

	9	C ₆ H ₁₄	Hexane	n-Hexane	
	10		2-Methylpentane	Isohexane	
	11		3-Methylpentane		
	12		2,2-Dimethylbutane	Neohexane	
	13		2,3-Dimethylbutane	Diisopropyl	
No.	9	10	11	12	13
T _f (deg.C)	-95	-154		-100	-129
d _f (kg/m ³)	759.	804.4		751.	787.
T			d		
deg.C			kg/m ³		
-150		801.0	815.		
-140		792.5	806.		
-130		784.1	797.		
-120		775.6	789.		779.
-110		767.1	780.		771.
-100		758.6	771.	751.	763.
-90	755.	750.1	763.	743.	755.
-80	747.	741.5	754.	735.	747.
-70	738.	733.0	745.	727.	739.
-60	730.	724.4	736.	719.	731.
-50	721.	715.7	728.	710.	722.
-40	712.	707.0	719.	702.	714.
-30	704.	698.2	710.	693.	706.
-20	695.	689.4	701.	685.	697.
-10	686.3	680.5	692.	676.	688.
0	677.4	671.5	683.	667.	679.6
10	668.4	662.3	673.7	658.2	670.7
20	659.37	653.09	664.40	649.04	661.69
30	650.16	643.7	655.0	639.7	652.5
40	640.82	634.1	645.	630.	643.2
50	631.32	624.4	636.	620.	633.7
60	621.63	614.5	626.	610.	623.9
70	611.74	604.3	616.	600.	613.9
80	601.62	593.8	605.	590.	603.6
90	591.22	583.0	594.	579.	593.1
100	580.51	571.9	583.	567.	582.1
110	569.4	560.4	572.	556.	570.8
120	558.0	548.3	560.	543.	559.0
130	546.0	535.7	548.	530.	546.6
140	533.4	522.4	535.	516.	533.5
150	520.2	508.3	521.	501.	519.7
160	506.1	493.	507.	485.	504.8
170	491.0	476.	491.	467.	488.7
180	474.	458.	473.	447.	471.0
190	456.	437.	454.	424.	451.0
200	435.	412.	432.	394.	428.
210	411.	381.	405.	350.	398.
220	379.	331.	368.		356.
230	329.		295.		
T _c (deg.C)	234.75	224.7	231.3	216.2	227.1
d _c (kg/m ³)	234.	236.	235.	248.	248.

TABLE 5(D)
SATURATED LIQUID DENSITY of C₇ ALKANES-I

Units: kg/m ³ v. deg.C				
14	C ₇ H ₁₆	Heptane	n-Heptane	
15		2-Methylhexane		
16		3-Methylhexane		
17		3-Ethylpentane	Triethylmethane	
No.	14	15	16	17
T _f (deg.C)	-91	-118		-119
d _f (kg/m ³)	776.	792.		815.
T	d			
deg.C	kg/m ³			
-110		785.	795.	807.
-100		777.	787.	799.
-90	775.	769.	778.	791.
-80	767.	761.	770.	783.
-70	759.	753.	762.	774.
-60	751.	745.	754.	766.
-50	742.	737.	746.	758.
-40	734.	729.	738.	749.
-30	726.	721.	729.	741.
-20	718.	712.	721.	733.
-10	709.4	704.	713.	724.
0	701.0	696.	704.	716.
10	692.6	687.2	695.8	706.9
20	684.06	678.68	687.20	698.23
30	675.46	670.02	678.51	689.48
40	666.77	661.3	669.7	680.6
50	657.96	652.4	660.8	671.6
60	649.02	643.3	651.8	662.5
70	639.9	634.1	642.5	653.3
80	630.7	624.7	633.2	643.9
90	621.3	615.1	623.6	634.3
100	611.7	605.3	613.8	624.5
110	601.8	595.2	603.7	614.5
120	591.7	584.7	593.4	604.2
130	581.3	574.0	582.7	593.6
140	570.5	562.8	571.7	582.6
150	559.3	551.	560.	571.
160	547.7	539.	548.	559.
170	535.4	526.	536.	547.
180	522.6	512.	522.	534.
190	508.9	498.	508.	520.
200	494.	482.	493.	505.
210	478.	464.	476.	489.
220	461.	444.	457.	471.
230	441.	421.	435.	451.
240	417.	392.	409.	427.
250	388.	350.	375.	398.
260	345.		311.	355.
T _c (deg.C)	267	257.2	262.1	267.5
d _c (kg/m ³)	236.	241.	241.	241.