Reviews

Vapor−Liquid Critical Properties of Elements and Compounds. 5. Branched Alkanes and Cycloalkanes

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This is part 5 of a series of contributions by the critical properties group of the IUPAC Commission 1.2 on Thermodynamics, Subcommittee on Thermodynamic Data. It presents all the known experimental data for the critical temperature, pressure, and volume of branched alkanes and cycloalkanes. Critical temperatures have been converted to the ITS-90 scale. Recommendations together with uncertainties are given for 54 compounds.

Introduction

This critical review covers known critical properties for 42 branched paraffins, 10 cycloparaffins, and the 2 bicyclo-[4.4.0]decanes (decalins). The presentation and criteria for evaluation of the experimental data follow the guidelines of part 1 of the series [95-amb/you] and are not reiterated in this paper. Previous articles in this series all of which contain specific recommended values for critical properties include the *n*-alkanes [95-amb/tso], the aromatic hydrocarbons [95-tso/amb], and the aliphatic alcohols [95-gud/tej].

Recommended values are summarized in Table 1, while all experimental data located have been tabulated in Table 2. References to all experimental data cited are given in the Literature Cited.

In the analysis of each compound to select the recommended value, compounds were grouped in families, when possible, in order to determine if trends were reasonable as the carbon number increased. Plots were made of critical temperature, pressure, volume, and compressibility factor against carbon number for compound families with four to seven carbon atoms. All recommended values are consistent with these plots, and comments relating to these analyses are given where appropriate.

Branched Alkanes

Experimental values for critical properties of 42 branched alkanes have been located, although extensive data are only available for certain four to seven carbon atom compounds.

Critical properties for 2-methylpropane have been measured by at least five investigators and have been thoroughly analyzed by several other investigators using equations of state. The values chosen are those agreed upon by Goodwin and Haynes [82-goo/hay] and Younglove and Ely [87-you/ely] in their extensive evaluations. However, the uncertainties are relatively high compared to many other branched alkanes because of disagreements in the earlier experimental work cited.

Experimental values for 2-methylbutane were measured by five investigators. The value of the critical temperature reported by Pawlewski [1883-paw] is high and close to the accepted value for pentane. The values of the critical temperature and pressure reported by Altschul [1893-alt] for "pentan" are included as they are closer to the values for 2-methylbutane than to those for pentane, where they are also listed by Ambrose and Tsonopoulos [95-amb/tso]. Das et al. [77-das/ree] accepted the critical temperature measured by Ambrose et al. [60-amb/cox], a critical pressure intermediate between the values measured by Young [10-you] and Vohra and Kobe [59-voh/kob], and the critical density from Vohra and Kobe. The values recommended by this study are in line with the previous evaluation. Uncertainties indicate the spread of the three reliable experimental data sources. Comparison of all the 2-methylalkanes by plotting suggests that the reported experimental critical pressure of 2-methylbutane may be slightly high. However, the selected value is deemed the most likely correct value on the basis of the experimental data available. 2,2-Dimethylpropane values all agree within experimental accuracy. The values chosen are averages of the published experimental values.

For all branched alkanes the recommended values were either taken as the latest value or the mean of several reliable values. Plots of properties of 2-methyl, 3-methyl, 2,2-dimethyl, and 2,3-dimethyl compounds against carbon number were made for each property to verify whether the chosen values were reasonable. Except for the critical compressibility factor, as is readily apparent from Table 1, the properties exhibited expected trends and are appropriately recommended.

For the four six-carbon-atom branched alkanes, all measurements since 1946 are reasonable and averages are recommended for each compound. As fewer data points from only three references exist for the eight seven-carbon-atom compounds, except for 2-methylhexane, the uncertainties in the critical temperature and pressure have been increased. Plots of the properties by family indicate that all properties are within the assigned uncertainties.

Most data for the sixteen eight-carbon-atom and the eleven nine- and ten-carbon-atom compounds are derived from one experimental source. For such compounds the uncertainties have been assigned to allow for greater error than in cases where several data sources were available.

0021-9568/96/1741-0365$12.00/0

Table 1. Recommended Values of Critical Properties of Branched Alkanes and Cycloalkanes

	M/g·mol^{-1}	T_c/K[a] (±)[b]	p_c/MPa (±)[b]	ρ_c/g·cm^{-3} (±)[b]	V_c/cm^3·mol^{-1}	Z_c[c]
2-methylpropane	58.123	407.8(0.5)	3.640(0.05)	0.224(0.003)	259	0.278
2-methylbutane	72.150	460.4(0.5)	3.38(0.05)	0.236(0.002)	306	0.270
2,2-dimethylpropane	72.150	433.8(0.1)	3.196(0.01)	0.235(0.003)	307	0.272
2-methylpentane	86.177	497.7(0.2)	3.04(0.02)	0.234(0.004)	368	0.270
3-methylpentane	86.177	504.6(0.2)	3.12(0.02)	0.234(0.004)	368	0.274
2,2-dimethylbutane	86.177	489.0(0.3)	3.10(0.02)	0.241(0.004)	358	0.279
2,3-dimethylbutane	86.177	500.0(0.2)	3.15(0.02)	0.239(0.004)	361	0.279
2-methylhexane	100.204	530.4(0.2)	2.74(0.02)	0.238(0.004)	421	0.262
3-methylhexane	100.204	535.2(0.4)	2.81(0.04)	0.248(0.004)	404	0.256
3-ethylpentane	100.204	540.6(0.4)	2.89(0.04)	0.241(0.004)	416	0.267
2,2-dimethylpentane	100.204	520.5(0.5)	2.77(0.05)	0.241(0.004)	416	0.266
2,3-dimethylpentane	100.204	537.3(0.5)	2.91(0.05)	0.255(0.004)	393	0.256
2,4-dimethylpentane	100.204	519.8(0.5)	2.74(0.05)	0.240(0.004)	418	0.265
3,3-dimethylpentane	100.204	536.4(0.5)	2.95(0.05)	0.242(0.004)	414	0.274
2,2,3-trimethylbutane	100.204	531.1(0.3)	2.95(0.05)	0.252(0.004)	398	0.265
2-methylheptane	114.231	559.7(0.1)	2.50(0.02)	0.234(0.002)	488	0.262
3-methylheptane	114.231	563.6(0.5)	2.55(0.04)	0.246(0.004)	464	0.253
4-methylheptane	114.231	561.7(0.5)	2.54(0.04)	0.240(0.004)	476	0.259
3-ethylhexane	114.231	565.5(0.5)	2.61(0.04)	0.251(0.004)	455	0.252
2,2-dimethylhexane	114.231	549.8(0.5)	2.53(0.04)	0.239(0.004)	478	0.265
2,3-dimethylhexane	114.231	563.5(0.5)	2.63(0.04)	0.244(0.004)	468	0.263
2,4-dimethylhexane	114.231	553.5(0.5)	2.56(0.04)	0.242(0.004)	472	0.263
2,5-dimethylhexane	114.231	550.0(0.5)	2.49(0.02)	0.237(0.002)	482	0.262
3,3-dimethylhexane	114.231	562.0(0.5)	2.65(0.04)	0.258(0.004)	443	0.251
3,4-dimethylhexane	114.231	568.8(0.5)	2.69(0.04)	0.245(0.004)	466	0.265
2-methyl-3-ethylpentane	114.231	567.1(0.5)	2.70(0.04)	0.258(0.004)	442	0.253
3-methyl-3-ethylpentane	114.231	576.5(0.5)	2.81(0.04)	0.251(0.004)	455	0.266
2,2,3-trimethylpentane	114.231	563.5(0.5)	2.73(0.04)	0.262(0.004)	436	0.254
2,2,4-trimethylpentane	114.231	543.8(0.3)	2.57(0.02)	0.244(0.002)	468	0.267
2,3,3-trimethylpentane	114.231	573.5(0.5)	2.82(0.04)	0.251(0.004)	455	0.269
2,3,4-trimethylpentane	114.231	566.4(0.5)	2.73(0.04)	0.248(0.004)	460	0.267
2-methyloctane	128.258	582.8(0.1)	2.31(0.02)			
2,2-dimethylheptane	128.258	576.7(0.5)	2.35(0.04)			
2,2,5-trimethylhexane	128.258	569.8(2.0)				
2,2,3,3-tetramethylpentane	128.258	607.5(0.5)	2.74(0.04)			
2,2,3,4-tetramethylpentane	128.258	592.6(0.5)	2.60(0.04)			
2,2,4,4-tetramethylpentane	128.258	574.6(0.5)	2.49(0.04)			
2,3,3,4-tetramethylpentane	128.258	607.5(0.5)	2.72(0.04)			
3,3,5-trimethylheptane	142.285	609.5(0.5)	2.32(0.04)			
2,2,3,3-tetramethylhexane	142.285	623.0(0.5)	2.51(0.04)			
2,2,5,5-tetramethylhexane	142.285	581.4(0.5)	2.19(0.04)			
2,2,4,4,6,8,8-heptamethylnonane	226.446	692(4)				
cyclopropane	42.081	398.0(0.3)	5.54(0.05)	0.259(0.004)	162	0.272
cyclopentane	70.134	511.7(0.2)	4.51(0.04)	0.270(0.004)	259	0.275
cyclohexane	84.161	553.8(0.2)	4.08(0.03)	0.273(0.002)	308	0.273
methylcyclopentane	84.161	532.7(0.2)	3.79(0.04)	0.264(0.004)	318	0.272
cycloheptane	98.188	604.2(0.5)	3.82(0.04)	0.278(0.005)	353	0.268
methylcyclohexane	98.188	572.1(0.2)	3.48(0.02)	0.266(0.002)	369	0.270
ethylcyclopentane	98.188	569.5(0.5)	3.40(0.04)	0.262(0.004)	375	0.269
cyclooctane	112.215	647.2(0.5)	3.56(0.04)	0.274(0.005)	410	0.271
trans-1,4-dimethylcyclohexane	112.215	587.7(0.5)				
r-1,*c*-3,*t*-5-trimethylcyclohexane	126.242	602.2(0.5)				
cis-bicyclo[4.4.0]decane	138.253	703.6(3)	3.2(0.2)			
trans-bicyclo[4.4.0]decane	138.253	687(3)				

[a] Temperatures are expressed on ITS-90. [b] The uncertainties (±) are based on minima set by the lower molecular weight compounds except when multiple values are available from experimental investigators. [c] $Z_c = P_cV_c/RT_c$ where $R = 8.314\ 51$ J·mol^{-1}·K^{-1}

Table 2. Critical Properties from the Literature

year	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
	2-METHYLPROPANE: molar mass 58.123 g; CASRN 75-28-5					
	$T_{68} - T_{48} = 0.01$ K, $T_{90} - T_{68} = -0.03$ K, $T_{90} - T_{48} = -0.02$ K at 407.80 K					
15-sei/bur	133.7 °C, 27771 mmHg	406.8	3.702		1	Seibert and Burrell
35-har	133.8 °C	407.0			1	Harand
40-gil/sch	274 °F, 535 psi	407.6	3.69		1, 5	Gilliland and Scheeline
49-bea/edw	134.98 °C, 36.00 atm	408.11	3.65	0.221	3	Beattie, Edwards, and Marple
62-con	134.62 °C, 35.85 atm	407.15	3.70			Connolly
73-das/ree	36.0 atm	408.1	3.65	0.221	8	Das, Reed, and Eubank
82-goo/hay		407.82	3.640	0.224	8	Goodwin and Haynes
83-wax/gal		407.82	3.6306	0.227	8	Waxman and Gallagher
83-lev/kam		407.81	3.629	0.2255	8	Levelt Sengers, Kamgar-Parsi, and Sengers
87-you/ely	3.860 mol·dm^{-3}	407.82	3.640	0.2244	8	Younglove and Ely
	recommended values	407.8 ± 0.5	3.640 ± 0.05	0.224 ± 0.003		

Table 2. (Continued)

year	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
	2-METHYLBUTANE: molar mass 72.150 g; CASRN 78-78-4					
1883-paw	194.8 °C	468.0			1	Pawlewski
1893-alt	187.1 °C, 33.3 kg·cm^{-2}	460.2	3.27		1	Altschul
1899-you, 10-you	87.8 °C, 25018 mmHg	460.95	3.33	0.2343	1	Young
59-voh/kob	187.8 °C, 33.66 atm	461.0	3.410	0.236	3	Vohra and Kobe
60-amb/cox	187.24 °C	460.39			1	Ambrose, Cox, and Townsend
77-das/ree	(33.37 ± 0.1) atm	460.39	3.381	0.236	8	Das, Reed, and Eubank
	recommended values	460.4 ± 0.5	3.38 ± 0.05	0.236 ± 0.002		
	2,2-DIMETHYLPROPANE: molar mass 72.150 g; CASRN 463-82-1					
51-bea/dou	160.60 °C, 31.57 atm, 0.303 L·mol^{-1}	433.74	3.199	0.238	3	Beattie, Douslin, and Levine
60-par/row	160.6 °C	433.8			1	Partington, Rowlinson, and Weston
73-daw/sil	(160 ± 0.05) °C, (31.545 ± 0.02) atm (4.312 ± 0.01) mL·g^{-1}	433.74	3.1963	0.2319	3	Dawson, Silberberg, and McKetta
77-das/ree	31.545 atm	433.74	3.1963	0.232	8	Das, Reed and Eubank
	recommended values	433.8 ± 0.1	3.196 ± 0.01	0.235 ± 0.003		
	2-METHYLPENTANE: molar mass 86.177 g; CASRN 107-83-5					
46-kay	224.7 °C, 29.95 atm	497.8	3.035	0.235	1a	Kay
60-amb/cox	224.30 °C	497.46			1	Ambrose, Cox, and Townsend
74-kay/you		497.81	3.031		1a	Kay and Young
75-kay/you		497.75	3.032		1a	Kay and Young
80-gen/tej	368.43 cm^3·mol^{-1}	497.79	3.032	0.2339	1a	Genco, Teja, and Kay
88-aba/jen		497.71	3.04		1c	Abara *et al.*
	recommended values	497.7 ± 0.2	3.04 ± 0.02	0.234 ± 0.004		
	3-METHYLPENTANE: molar mass 86.177 g; CASRN 96-14-0					
46-kay	231.2 °C, 30.83 atm	504.4	3.124	0.235	1a	Kay
52-day/fel	231.5 °C, 30.75 atm	504.6	3.116		3, 4	Day and Felsing
74-you		504.4			1	Young
74-kay/you		504.58	3.128		1a	Kay and Young
75-kay/you		504.55	3.124		1a	Kay and Young
80-gen/tej	368.71 cm^3·mol^{-1}	504.56	3.1244	0.2337	1a	Genco, Teja, and Kay
	recommended values	504.6 ± 0.2	3.12 ± 0.02	0.234 ± 0.004		
	2,2-DIMETHYLBUTANE: molar mass 86.177 g; CASRN 75-83-2					
46-kay	216.2 °C, 30.67 atm	489.4	3.108	0.240	1a	Kay
60-amb/cox	215.58 °C	488.74			1	Ambrose, Cox, and Townsend
74-you		488.7			1	Young
75-kay/you		489.20	3.102		1a	Kay and Young
80-gen/tej	358.10 cm^3·mol^{-1}	489.21	3.1024	0.2407	1a	Genco, Teja, and Kay
	recommended values	489.0 ± 0.3	3.10 ± 0.02	0.241 ± 0.004		
	2,3-DIMETHYLBUTANE: molar mass 86.177 g; CASRN 79-29-8					
00-you/for, 10-you	227.35 °C, 23360 mmHg	500.5	3.115	0.2411	1	Young and Fortey
46-kay	227.1 °C, 30.99 atm	500.2	3.140	0.241	1a	Kay
60-amb/cox	226.78 °C	499.94			1	Ambrose, Cox, and Townsend
74-you		499.9			1	Young
74-kay/you		500.19	3.147		1a	Kay and Young
75-kay/you		500.08	3.145		1a	Kay and Young
80-gen/tej	360.15 cm^3·mol^{-1}	500.04	3.1452	0.2393	1a	Genco, Teja, and Kay
92-qua/kud		499.8	3.18		1a	Quadri and Kudchadker
	recommended values	500.0 ± 0.2	3.15 ± 0.02	0.239 ± 0.004		
	2-METHYLHEXANE: molar mass 100.204 g; CASRN 591-76-4					
29-edg/cal	257.9 °C, 27.2 atm	531.0	2.76		3	Edgar and Calingaert
60-amb/cox	257.18 °C	530.36			1	Ambrose, Cox, and Townsend
65-mcm/kay	257.15 °C, 26.971 atm	530.33	2.7328	0.238	1a	McMicking and Kay
88-aba/jen		530.39	2.750		1a	Abara *et al.*
	recommended values	530.4 ± 0.2	2.74 ± 0.02	0.238 ± 0.004		
	3-METHYLHEXANE: molar mass 100.204 g; CASRN 589-34-4					
29-edg/cal	262.4 °C, 28.1 atm	535.6	2.85		3	Edgar and Calingaert
65-mcm/kay	262.04 °C, 27.767 atm	535.22	2.8135	0.248	1a	McMicking and Kay
	recommended values	535.2 ± 0.4	2.81 ± 0.04	0.248 ± 0.004		
	3-ETHYLPENTANE: molar mass 100.204 g; CASRN 617-78-7					
29-edg/cal	267.6 °C, 28.6 atm	540.8	2.90		3	Edgar and Calingaert
65-mcm/kay	267.42 °C, 28.530 atm	540.60	2.8908	0.241	1a	McMicking and Kay
	recommended values	540.6 ± 0.4	2.89 ± 0.04	0.241 ± 0.004		

Table 2. (Continued)

year	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
	2,2-DIMETHYLPENTANE: molar mass 100.204 g; CASRN 590-35-2					
29-edg/cal	247.7 °C, 28.4 atm	520.8	2.88		3	Edgar and Calingaert
65-mcm/kay	247.29 °C, 27.367 atm	520.47	2.7730	0.241	1a	McMicking and Kay
	recommended values	520.5 ± 0.5	2.77 ± 0.05	0.241 ± 0.004		
	2,3-DIMETHYLPENTANE: molar mass 100.204 g; CASRN 565-59-3					
29-edg/cal	264.6 °C, 29.2 atm	537.8	2.97		3	Edgar and Calingaert
57-fra	264. °C	537.			1	Francis
65-mcm/kay	264.14 °C, 28.700 atm	537.32	2.9080	0.255	1a	McMicking and Kay
	recommended values	537.3 ± 0.5	2.91 ± 0.05	0.255 ± 0.004		
	2,4-DIMETHYLPENTANE: molar mass 100.204 g; CASRN 108-68-7					
29-edg/cal	247.1 °C, 27.4 atm	520.2	2.78		3	Edgar and Calingaert
57-fra	248.5 °C	521.6			1	Francis
65-mcm/kay	246.58 °C, 27.009 atm	519.76	2.7367	0.240	1a	McMicking and Kay
	recommended values	519.8 ± 0.5	2.74 ± 0.05	0.240 ± 0.004		
	3,3-DIMETHYLPENTANE: molar mass 100.204 g; CASRN 562-49-2					
65-mcm/kay	263.19 °C, 29.073 atm	536.37	2.9458	0.242	1a	McMicking and Kay
	recommended values	536.4 ± 0.5	2.95 ± 0.05	0.242 ± 0.004		
	2,2,3-TRIMETHYLBUTANE: molar mass 100.204 g; CASRN 464−06−2					
29-edg/cal	258.3 °C, 29.75 atm	531.4	3.014		3	Edgar and Calingaert
65-mcm/kay	257.96 °C, 29.146 atm	531.13	2.9532	0.252	1a	McMicking and Kay
	recommended values	531.1 ± 0.3	2.95 ± 0.05	0.252 ± 0.004		
	2-METHYLHEPTANE: molar mass 114.231 g; CASRN 592-27-8					
60-amb/cox	286.42 °C	559.60			1	Ambrose, Cox, and Townsend
65-mcm/kay	286.41 °C, 24.517 atm	559.59	2.4842	0.234	1a	McMicking and Kay
88-aba/jen		559.66	2.50		1c	Abara *et al.*
	recommended values	559.7 ± 0.1	2.50 ± 0.02	0.234 ± 0.002		
	3-METHYLHEPTANE: molar mass 114.231 g; CASRN 589-81-1					
65-mcm/kay	290.45 °C, 25.127 atm	563.63	2.5460	0.246	1a	McMicking and Kay
	recommended values	563.6 ± 0.5	2.55 ± 0.04	0.246 ± 0.004		
	4-METHYLHEPTANE: molar mass 114.231 g; CASRN 589-53-7					
65-mcm/kay	288.52 °C, 25.087 atm	561.70	2.5419	0.240	1a	McMicking and Kay
	recommended values	561.7 ± 0.5	2.54 ± 0.04	0.240 ± 0.004		
	3-ETHYLHEXANE: molar mass 114.231 g; CASRN 619-99-8					
65-mcm/kay	292.27 °C, 25.738 atm	565.45	2.6079	0.251	1a	McMicking and Kay
	recommended values	565.5 ± 0.5	2.61 ± 0.04	0.251 ± 0.004		
	2,2-DIMETHYLHEXANE: molar mass 114.231 g; CASRN 590-73-8					
65-mcm/kay	276.65 °C, 24.961 atm	549.83	2.5292	0.239	1a	McMicking and Kay
	recommended values	549.8 ± 0.5	2.53 ± 0.04	0.239 ± 0.004		
	2,3-DIMETHYLHEXANE: molar mass 114.231 g; CASRN 584-94-1					
65-mcm/kay	290.27 °C, 25.938 atm	563.45	2.6282	0.244	1a	McMicking and Kay
	recommended values	563.5 ± 0.5	2.63 ± 0.04	0.244 ± 0.004		
	2,4-DIMETHYLHEXANE: molar mass 114.231 g; CASRN 589-43-5					
65-mcm/kay	280.30 °C, 25.229 atm	553.48	2.5566	0.242	1a	McMicking and Kay
	recommended values	553.5 ± 0.5	2.56 ± 0.04	0.242 ± 0.004		
	2,5-DIMETHYLHEXANE: molar mass 114.231 g; CASRN 592−13−2					
1883-paw	270.8 °C	544.0			1	Pawlewski
00-you/for, 10-you	276.8 °C, 18 660 mmHg	550.0	2.488	0.2366	1	Young and Fortey
65-mcm/kay	276.84 °C, 24.542 atm	550.02	2.4867	0.237	1a	McMicking and Kay
	recommended values	550.0 ± 0.5	2.49 ± 0.02	0.237 ± 0.002		
	3,3-DIMETHYLHEXANE: molar mass 114.231 g; CASRN 563-16-6					
65-mcm/kay	288.80 °C, 26.187 atm	561.98	2.6534	0.258	1a	McMicking and Kay
	recommended values	562.0 ± 0.5	2.65 ± 0.04	0.258 ± 0.004		
	3,4-DIMETHYLHEXANE: molar mass 114.231 g; CASRN 583-48-2					
65-mcm/kay	295.63 °C, 26.569 atm	568.81	2.6921	0.245	1a	McMicking and Kay
	recommended values	568.8 ± 0.5	2.69 ± 0.04	0.245 ± 0.004		
	2-METHYL-3-ETHYLPENTANE: molar mass 114.231 g; CASRN 609-26-7					
65-mcm/kay	293.87 °C, 26.651 atm	567.05	2.7004	0.258	1a	McMicking and Kay
	recommended values	567.1 ± 0.5	2.70 ± 0.04	0.258 ± 0.004		
	3-METHYL-3-ETHYLPENTANE: molar mass 114.231 g; CASRN 1067-08-9					
65-mcm/kay	303.36 °C, 27.706 atm	576.54	2.8073	0.251	1a	McMicking and Kay
	recommended values	576.5 ± 0.5	2.81 ± 0.04	0.251 ± 0.004		

Table 2. (Continued)

year	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
	2,2,3-TRIMETHYLPENTANE: molar mass 114.231 g; CASRN 564-02-3					
65-mcm/kay	290.28 °C, 26.937 atm	563.46	2.7294	0.262	1a	McMicking and Kay
	recommended values	563.5 ± 0.5	2.73 ± 0.04	0.262 ± 0.004		
	2,2,4-TRIMETHYLPENTANE: molar mass 114.231 g; CASRN 540-84-1					
48-bea/edw	(271.15 ± 0.01) °C, (25.5 ± 0.10) atm	544.33	2.58	0.237 ± 3%	3	Beattie and Edwards
51-kay/war	270.676 °C, 25.308 atm	543.853	2.5643	0.243	1a	Kay and Warzel
60-amb/cox	(270.46 ± 0.03) °C	543.6			1	Ambrose, Cox, and Townsend
65-mcm/kay	270.74 °C, 25.340 atm	543.92	2.5676	0.244	1a	McMicking and Kay
	recommended values	543.8 ± 0.3	2.57 ± 0.02	0.244 ± 0.002		
	2,3,3-TRIMETHYLPENTANE: molar mass 114.231 g; CASRN 560-21-4					
65-mcm/kay	300.34 °C, 27.833 atm	573.52	2.8202	0.251	1a	McMicking and Kay
	recommended values	573.5 ± 0.5	2.82 ± 0.04	0.251 ± 0.004		
	2,3,4-TRIMETHYLPENTANE: molar mass 114.231 g; CASRN 565-75-3					
65-mcm/kay	293.19 °C, 26.941 atm	566.37	2.7298	0.248	1a	McMicking and Kay
	recommended values	566.4 ± 0.5	2.73 ± 0.04	0.248 ± 0.004		
	2-METHYLOCTANE: molar mass 128.258 g; CASRN 3221-61-2					
69-kay/his	309.72 °C, 335 psia	582.83	2.31		1	Kay and Hissong
88-aba/jen	582.87 K, 2.31 MPa	582.83	2.310		1c	Abara *et al.*
	recommended values	582.8 ± 0.1	2.31 ± 0.02			
	2,2-DIMETHYLHEPTANE: molar mass 128.258 g; CASRN 1071-26-7					
69-kay/his	303.54 °C, 340.8 psia	576.65	2.349		1	Kay and Hissong
	recommended values	576.7 ± 0.5	2.35 ± 0.04			
	2,2,5-TRIMETHYLHEXANE: molar mass 128.258 g; CASRN 3522-94-9					
57-fra	296.7 °C	569.8			1	Francis
	recommended value	569.8 ± 2.0				
	2,2,3,3-TETRAMETHYLPENTANE: molar mass 128.258 g; CASRN 7154-79-2					
68-amb/tow	(334.4 ± 0.1) °C	607.5	2.741		1	Ambrose and Townsend
	recommended values	607.5 ± 0.5	2.74 ± 0.04			
	2,2,3,4-TETRAMETHYLPENTANE: molar mass 128.258 g; CASRN 1186-53-4					
68-amb/tow	(319.5 ± 0.05) °C	592.61	2.602		1	Ambrose and Townsend
	recommended values	592.6 ± 0.5	2.60 ± 0.04			
	2,2,4,4-TETRAMETHYLPENTANE: molar mass 128.258 g; CASRN 1070-87-7					
68-amb/tow	(301.5 ± 0.05) °C	574.61	2.485		1	Ambrose and Townsend
	recommended values	574.6 ± 0.5	2.49 ± 0.04			
	2,3,3,4-TETRAMETHYLPENTANE: molar mass 128.258 g; CASRN 16747-38-9					
68-amb/tow	(334.4 ± 0.5) °C	607.5	2.716		1	Ambrose and Townsend
	recommended values	607.5 ± 0.5	2.72 ± 0.04			
	3,3,5-TRIMETHYLHEPTANE: molar mass 142.285 g; CASRN 7154−80−5					
68-amb/tow	(336.4 ± 0.5) °C	609.5	2.317		1	Ambrose and Townsend
	recommended values	609.5 ± 0.5	2.32 ± 0.04			
	2,2,3,3-TETRAMETHYLHEXANE: molar mass 142.285 g; CASRN 13475-81-5					
68-amb/tow	(349.9 ± 0.2) °C	623.0	2.51		1	Ambrose and Townsend
	recommended values	623.0 ± 0.5	2.51 ± 0.04			
	2,2,5,5-TETRAMETHYLHEXANE: molar mass 142.285 g; CASRN 1071-81-4					
68-amb/tow	(308.3 ± 0.5) °C	581.4	2.186		1	Ambrose and Townsend
	recommended values	581.4 ± 0.5	2.19 ± 0.04			
	2,2,4,4,6,8,8-HEPTAMETHYLNONANE: molar mass 226.446 g; CASRN 4930-04-9					
88-amb/ghi		692			1	Ambrose and Ghiassee
	recommended value	692 ± 4				
	CYCLOPROPANE: molar mass 42.081; CASRN 75-19-4					
58-boo/mor	124.65 °C, 54.23 atm	397.78	5.495		1	Booth and Morris
70-lin/sil	125.15 °C, 55.065 atm, 3.868 mL·g^{-1}	398.27	5.5795	0.2585	3	Lin, Silberberg, and McKetta
	recommended values	398.0 ± 0.3	5.54 ± 0.05	0.259 ± 0.004		
	CYCLOPENTANE: molar mass 70.134 g; CASRN 287-92-3					
47-kay	238.60 °C, 44.550 atm	511.79	4.5140	0.270	1	Kay
57-amb/gra	(238.4 ± 0.02) °C	511.5			1	Ambrose and Grant
68-kud/ala	238.5 °C, 44.49 atm	511.6	4.508	0.27	10	Kudchadker, Alani, and Zwolinski
	recommended values	511.7 ± 0.2	4.51 ± 0.04	0.270 ± 0.004		

Table 2. (Continued)

year	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
	METHYLCYCLOPENTANE: molar mass 84.161 g; CASRN 96-37-7					
47-kay	259.61 °C, 37.364 atm	532.79	3.7859	0.264	1	Kay
60-amb/cox	259.55 °C	532.73			1	Ambrose, Cox, and Townsend
68-kud/ala	259.58 °C, 37.35 atm	532.69	3.784	0.264	10	Kudchadker, Alani, and Zwolinski
	recommended values	532.7 ± 0.2	3.79 ± 0.04	0.264 ± 0.004		
	CYCLOHEXANE: molar mass 84.161 g; CASRN 110-82-7					
1899-you						
10-you	280 °C, 30278 mmHg	553	4.034	0.2735	1	Young
34-rot/nag	281.0 °C, 40.57 atm	554.1	4.111	0.2725	1	Rotinjanz and Nagornow
43-fis/rei	280.7 °C	553.8			1	Fischer and Reichel
56-kay/alb	535.64 °F, 591.5 psia	552.98	4.078		1	Kay and Albert
57-sim	280.2 °C	553.3		0.2718	1, 7	Simon
57-gla/rue	281 °C, 40.57 atm	554	4.111		3	Glaser and Rüland
57-amb/gra	(280.3 ± 0.02) °C	553.4			1	Ambrose and Grant
59-ric/row	(280.2 ± 0.05) °C	553.3			1	Richardson and Rowlinson
60-par/row	280.2 °C	553.3			1	Partington, Rowlinson, and Weston
63-che	(280.2 ± 0.1) °C	553.3			1	Cheng
72-you	309 cm^3·mol^{-1}		4.036	0.272	1	Young
72-pak/kay	279.8 °C, 594.2 psia	552.9	4.097		1	Pak and Kay
72-rae/str		555.1			1	Rätzsch and Strauch
78-hug/mcg		553.60	4.075		1	Hugill and McGlashan
90-tej/ros		553.7	4.071		1	Teja and Rosenthal
90-tej/ans		553.9		0.274	1	Teja and Anselme
	recommended values	553.8 ± 0.2	4.08 ± 0.03	0.273 ± 0.002		
	CYCLOHEPTANE: molar mass 98.188 g; CASRN 291-64-5					
71-hic/you	37.76 atm	604.2	3.83		1	Hicks and Young
72-you	353 cm^3·mol^{-1}	604.3	3.81	0.278	1	Young
	recommended values	604.2 ± 0.5	3.82 ± 0.04	0.278 ± 0.005		
	METHYLCYCLOHEXANE: molar mass 98.188 g; CASRN 108-87-2					
26-nag/rot	301.5 °C				1	Nagornow and Rotinjanz
47-kay	299.13 °C	572.31	3.4777	0.285	1	Kay
57-fra	300 °C	573.			1	Francis
57-sim	299.5 °C	572.6		0.2666	1, 7	Simon
60-amb/cox	298.97 °C	572.15			1	Ambrose, Cox, and Townsend
68-kud/ala	298.97 °C, 34.26 atm	572.15	3.471	0.267	10	Kudchadker, Alani, and Zwolinski
70-pow/swi		572.16			1	Powell, Swinton, and Young
	recommended values	572.1 ± 0.2	3.48 ± 0.02	0.266 ± 0.002		
	ETHYLCYCLOPENTANE: molar mass 98.188 g; CASRN 1640-89-7					
47-kay	296.30 °C, 33.526 atm	569.48	3.3970	0.262	1	Kay
	recommended values	569.5 ± 0.5	3.40 ± 0.04	0.262 ± 0.004		
	CYCLOOCTANE: molar mass 112.215 g; CASRN 292-64-8					
71-hic/you	35.1 atm	647.2	3.56		1	Hicks and Young
72-you	410 cm^3·mol^{-1}		3.55	0.274	1	Young
	recommended values	647.2 ± 0.5	3.56 ± 0.04	0.274 ± 0.005		
	trans-1,4-DIMETHYLCYCLOHEXANE: molar mass 112.215 g; CASRN 2207-04-7					
70-pow/swi		587.7			1	Powell, Swinton, and Young
	recommended value	587.7 ± 0.5				
	r-1,*c*-3,*t*-5-TRIMETHYLCYCLOHEXANE: molar mass 126.242 g; CASRN 179-27-3					
70-pow/swi		602.2			1	Powell, Swinton, and Young
	recommended value	602.2 ± 0.5				
	cis-BICYCLO[4.4.0]DECANE: molar mass 138.253 g; CASRN 493-01-6					
57-gla/rue	372 °C, 20.5 atm	645	2.08		3	Glaser and Rüland
62-che/mcc		702.2			1	Cheng, McCoubrey, and Phillips
72-pak/kay	(431.8 ± 0.7) °C, (465.1 ± 2) psia	704.9	3.207		1	Pak and Kay
	recommended values	703.6 ± 3	3.2 ± 0.2			
	trans-BICYCLO[4.4.0]DECANE: molar mass 138.253 g; CASRN 493-02-7					
62-che/mcc		687.0			1	Cheng, McCoubrey, and Phillips
	recommended value	687 ± 3				

Cycloalkanes

Only 10 cycloalkanes have any experimental critical properties recorded. For cyclopropane and cyclopentane means of the experimental values were selected. For cyclohexane the mean of the Teja and Rosenthal [90-tej/ros] and Teja and Anselme [90-tej/ans] values by two

Table 3. Key to Methods of Critical Point Determination (Reprinted with Permission from 95-amb/you. Copyright 1995 American Chemical Society)

1.	visuals—in glass tube
2.	visuals—in cell with windows
3.	nonvisuals—*pVT* measurement
4.	other nonvisual measurement
5.	critical pressure measurements combined with vapor pressure measurements up to the critical point
6.	critical pressure by extrapolation of vapor pressure curve
7.	orthobaric density measurements
8.	equation of state, thermodynamic study
9.	calculation from another physical property
10.	literature survey
(a)	with stirring
(b)	instrumental detection of critical point
(c)	special feature of apparatus

different methods was taken for the critical temperature. The mean from the works of Young [72-you], Pak and Kay [72-pak/kay], and Teja and Rosenthal [90-tej/ros] was takenfor the critical pressure, while the critical density was taken from Teja and Anselme [90-tej/ans]. Mean values of critical pressure and critical density were taken for both cycloheptane and cyclooctane. For substituted cyclohexanes and cyclopentanes, average values of experimental measurements were used.

For *cis*-bicyclo[4.4.0]decane (*cis*-decalin or decahydronaphthalene) the average of Cheng et al. [62-che/mcc] and Pak and Kay [72-pak/kay] values were selected for the critical temperature. The Glaser and Rüland [57-gla/rue] values were ignored, as the values of both the critical temperature and the critical pressure appear low; the normal boiling point reported in Glaser and Rüland's work is closer to that of *cis*-bicyclo[4.4.0]decane, and the sample was probably a *cis/trans* mixture.

Acknowledgment

The author wishes to acknowledge Dr. Douglas Ambrose (University College, London, England) and Dr. Costa Tsonopoulos (Exxon Research and Engineering Co.) for their detailed review and guidance in this work.

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Received for review June 30, 1995. Accepted February 1, 1996.[⊗]

JE9501548

[⊗] Abstract published in *Advance ACS Abstracts*, March 15, 1996.