Reviews

Vapor−Liquid Critical Properties of Elements and Compounds. 11. Organic Compounds Containing B + O; Halogens + N, + O, + O + S, + S, + Si; N + O; and O + S, + Si

Douglas Ambrose

9 The Crest, Surbiton, Surrey KT5 8JZ, England

Constantine Tsonopoulos*

18 Dorothy Drive, Morristown, New Jersey 07960

Eugene D. Nikitin

Institute of Thermal Physics, Ural Branch of the Russian Academy of Sciences, Amundsena Street 106, 620016 Ekaterinburg, Russia

This review is part 11 of a series of contributions by the critical properties group of the previous IUPAC Commission I.2 on Thermodynamics, Subcommittee on Thermodynamic Data and the present IUPAC Project #2000-026-1-100, Critical Compilation of Vapor Liquid Critical Properties, sponsored by the Physical and Biophysical Chemistry Division. It presents all known experimental data for the critical constants of organic compounds containing at least two of the following atoms: B, Halogens (counted as one), N, O, S, and Si. Recommendations are given together with uncertainties. Critical temperatures have been converted, where warranted, to the ITS-90 scale.

Introduction

Part 11 completes the evaluation of experimental data for the critical properties of organic compounds by examining compounds containing two or more "heteroatoms" (halogens counted as one). Experimental data were found for 140 organic compounds containing the following combinations of heteroatoms: B + O (1); halogens + N (9); halogens + O (74); halogens + O + S (1); halogens + S (2); halogens + Si (5); N + O (15); O + S (2); and O + Si (31). The presentation and evaluation of the experimental data follow the guidelines of Ambrose et al. in parts 1 and 2 of this series: [95-amb/you] (introductory survey) and [95-amb/tso] (normal alkanes). Succeeding parts have been by Tsonopoulos and Ambrose [95-tso/amb] (aromatic hydrocarbons), Gude and Teja [95-gud/tej] (aliphatic alkanols), Daubert [96-dau] (branched alkanes and cycloalkanes), Tsonopoulos and Ambrose [96-tso/amb] (unsaturated aliphatic hydrocarbons), Kudchadker et al. [2001-kud/amb] (oxygen compounds other than alkanols and cycloalkanols), Tsonopoulos and Ambrose [2001-tso/amb] (organic sulfur, silicon, and tin compounds), Marsh et al. [2006-mar/you] (organic nitrogen compounds), and Marsh et al. [2007-mar/abr] (organic halogen compounds).

The recommended values are given in Table 1, while all known data have been collected in Table 2. Within a group, the compounds are listed in the order used by the Chemical Abstracts (Hill order). Additional values presented in Table 3 are not considered to satisfy the minimum requirement of having an experimentally determined T_c (see below) and are therefore not included in our recommendations in Table 1. The key to methods of critical point determination is presented in Table 4. Where appropriate, the data on which recommended values are based are indicated by an asterisk. Critical temperatures enclosed in parentheses are not new measurements; they are the values at which investigators determined the critical pressure (with method 5 or 6) and/or the critical density (with method 7 or 9). The references follow the format [year-first three letters of first author/first three letters of second author and, where required, a sequence number]. All four digits are given for the year starting with 2000 (as was also done in earlier parts for pre-1900 sources).

Uncertainties given in Table 2 are those given by authors or have been inferred from related work. As noted in earlier parts, such uncertainties are qualitative and frequently have low estimates. The uncertainties we give in the recommended values in Table 2 (and in Table 1) are generally greater than those appearing with each experimental value in Table 2. When only a single investigation has been made, which is true of the majority of the compounds in part 11, the recommendations are given only in Table 1. Generally, we have adjusted upward the uncertainties given by the authors for single investigations to bring them in line with the uncertainties for compounds investigated by several authors using a variety of techniques, including compounds examined in earlier parts of this series. In addition, we have tried to take into account information on the purity of the compound (before and after the measurement), relative merits of the technique used, and, in a few cases, the reputation of the laboratory and its investigators.

* Corresponding author. E-mail: ctsonop@verizon.net.

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Table 1. Recommended Critical Properties of Organic Compounds Containing B + O; Halogens + N, + O, + O +S, + S, + Si; N + O; and O + S, + Si

	molar mass M	T_c		p_c		ρ_c		V_c	
	$g \cdot mol^{-1}$ [a]	K [b]	(±)	MPa	(±)	$g \cdot cm^{-3}$	(±)	$cm^3 \cdot mol^{-1}$	Z_c [c]
B + O									
boric acid trimethyl ester	103.913	502	(1)	3.5	(0.1)				
Halogens + N									
trifluoroethanenitrile	95.023	311.1	(0.2)	3.62	(0.02)	0.47	(0.05)	202	0.283
difluoro-*N,N*-bis(trifluoromethyl)methanamine	203.034	404.94	(0.05)	2.727	(0.005)	0.591	(0.005)	344	0.278
N,N-bis(trifluoromethyl)methanamine	167.053	415.76	(0.05)	2.916	(0.005)	0.536	(0.005)	312	0.263
2,2-difluoro-*N,N*-bis(trifluoromethyl)ethanamine	217.061	460.20	(0.05)	2.642	(0.005)	0.579	(0.005)	375	0.259
N,N-bis(trifluoromethyl)ethanamine	181.080	442.60	(0.05)	2.622	(0.005)	0.490	(0.005)	370	0.263
1,1,2,2,3,3,3-heptafluoro-*N,N*-bis(heptafluoropropyl)-1-propanamine	521.069	524	(8)	1.35	(0.10)				
1,1,2,2,3,3,4,4,4-nonafluoro-*N*-nonafluorobutyl-*N*-(trifluoromethyl)-1-butanamine	521.069	530	(8)	1.36	(0.10)				
2,2,3,3,4,4,4a,5,5,6,6,7,7,8,8,8a-hexadecafluorodecahydro-1-(pentafluoroethyl)quinoline	545.091	575	(9)	1.61	(0.10)				
1,1,2,2,3,3,4,4,4-nonafluoro-*N,N*-bis(nonafluorobutyl)-1-butanamine	671.092	565.4	(0.5)	1.16	(0.05)				
Halogens + O									
trichloroacetyl chloride	181.833	605	(2)	4.3	(0.2)	0.53	(0.05)	343	0.293
trifluoroethanoic acid	114.023	491.3	(0.2)	3.258	(0.020)	0.559	(0.006)	204	0.163
difluoromethoxytrifluoromethane	136.021	354.49	(0.05)	3.351	(0.005)	0.579	(0.010)	235	0.267
oxy-bis(difluoromethane)	118.030	420.25	(0.05)	4.23	(0.10)	0.529	(0.010)	223	0.270
2,2,2-trifluoroethanol	100.040	498.5	(0.1)	4.825	(0.010)	0.485	(0.005)	206	0.240
trifluoromethoxymethane	100.040	377.92	(0.10)	3.635	(0.010)	0.462	(0.010)	217	0.250
chloropentafluoro-2-propanone	182.477	410.6	(0.5)	2.88	(0.05)				
hexafluorooxetane	166.022	361.9	(0.5)	3.06	(0.05)	0.610	(0.010)	272	0.277
hexafluoro-2-propanone	166.022	357.2	(0.5)	2.84	(0.05)	0.54	(0.05)	307	0.294
trifluoro(trifluoromethyl)oxirane	166.022	359.6	(0.2)	2.93	(0.02)	0.570	(0.011)	291	0.285
hexafluoro-1,3-dioxolane	182.021	368.1	(0.5)	2.71	(0.05)				
pentafluoro(trifluoromethoxy)ethane	204.019	356.8	(0.5)			0.640	(0.01)	319	
difluoro-bis(trifluoromethoxy)methane	220.018	372.4	(0.5)	2.33	(0.05)	0.61	(0.01)	361	0.271
1,1,1,2-tetrafluoro-2-(trifluoromethoxy)ethane	186.028	377.26	(0.05)	2.621	(0.005)	0.580	(0.005)	321	0.268
1,1,2,2-tetrafluoro-1-(trifluoromethoxy)ethane	186.028	387.8	(0.2)	2.62	(0.05)	0.55	(0.01)	338	0.275
2-chloro-1-(difluoromethoxy)-1,1,2-trifluoroethane	184.492	474.99	(0.05)	2.980	(0.005)				
2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane	184.492	467.76	(0.05)	3.046	(0.005)				
1,1,1-trifluoro-2-(trifluoromethoxy)ethane	168.038	401.90	(0.10)	2.856	(0.010)				
1,1,1,2-tetrafluoro-2-(difluoromethoxy)ethane	168.038	428.90	(0.10)	3.042	(0.010)	0.533	(0.005)	315	0.269
1,1,1-trifluoro-2-(difluoromethoxy)ethane	150.047	443.99	(0.05)	3.05	(0.10)				
1,2,2-trifluoro-2-(difluoromethoxy)ethane	150.047	462.03	(0.05)	3.538	(0.005)	0.533	(0.005)	282	0.259
pentafluoro(methoxy)ethane	150.047	406.82	(0.05)	2.886	(0.005)	0.500	(0.010)	300	0.256
2,2,3,3-tetrafluoro-1-propanol	132.057	553.6	(1.0)	4.63	(0.10)	0.496	(0.010)	266	0.268
carbonchloridic acid ethyl ester	108.524	<508	(?)						
1,1,1-trifluoro-2-(methoxy)ethane	114.066	449.05	(0.10)	3.509	(0.010)	0.412	(0.005)	277	0.260
octafluorotetrahydrofuran	216.029	400.0	(0.5)	2.69	(0.05)	0.68	(0.01)	318	0.257
1,1,1,2,2,3,3-heptafluoro-3-(trifluoromethoxy)propane	254.026	391.7	(0.5)	1.87	(0.05)	0.63	(0.01)	403	0.232
2,2,3,3,5,5,6-heptafluoro-1,4-dioxane	214.038	452.88	(0.05)	2.866	(0.005)	0.597	(0.005)	359	0.273
4,4,5,5-tetrafluoro-2-(trifluoromethyl)-1,3-dioxolane	214.038	435.06	(0.05)	2.645	(0.005)	0.569	(0.005)	376	0.275
pentafluoro(1,1,2,2-tetrafluoroethoxy)ethane	236.036	412.63	(0.05)	2.257	(0.005)	0.499	(0.005)	473	0.311
pentafluoro(2,2,2-trifluoroethoxy)ethane	218.045	421.60	(0.10)	2.327	(0.010)	0.533	(0.005)	409	0.272
1,1,1,3,3,3-hexafluoro-2-(difluoromethoxy)propane	218.045	444.63	(0.05)	2.571	(0.005)	0.581	(0.005)	375	0.261
1,1-bis(difluoromethoxy)-1,2,2,2-tetrafluoroethane	234.045	449.81	(0.05)	2.421	(0.005)	0.571	(0.005)	410	0.265
3,3,4,4,4-pentafluoro-2-butanone	162.058	453.03	(0.05)	2.912	(0.005)	0.486	(0.005)	333	0.258
3-difluoromethoxy-1,1,1,2,2-pentafluoropropane	200.055	455.10	(0.10)	2.773	(0.010)	0.576	(0.005)	347	0.255
1,1,1,2,2,3,3-heptafluoro-3-(methoxy)propane	200.055	437.60	(0.10)	2.480	(0.010)	0.530	(0.005)	377	0.257
1,1,1,2,3,3,3-heptafluoro-2-(methoxy)propane	200.055	433.21	(0.10)	2.548	(0.010)	0.542	(0.005)	369	0.261
1,1,2,2-tetrafluoro-1-(2,2,2-trifluoroethoxy)ethane	200.055	463.89	(0.05)	2.713	(0.005)	0.541	(0.005)	370	0.260
1,1,1,3,3,3-hexafluoro-2-(methoxy)propane	182.064	459.60	(0.10)	2.696	(0.010)	0.481	(0.005)	379	0.267
1,1,2,2-tetrafluoro-2-(2,2-difluoroethoxy)ethane	182.064	501.08	(0.05)	3.090	(0.005)	0.520	(0.005)	350	0.260
1,1,1-trifluoro-2-(2,2,2-trifluoroethoxy)ethane	182.064	476.31	(0.05)	2.783	(0.005)	0.500	(0.005)	364	0.256
pentafluoro(ethoxy)ethane	164.074	431.13	(0.10)	2.526	(0.010)	0.448	(0.005)	366	0.258
3-methoxy-1,1,2,2-tetrafluoropropane	146.083	505.35	(0.05)	3.279	(0.005)	0.453	(0.005)	322	0.252
nonafluoropentanoyl fluoride	266.037	427	(3)	1.90	(0.10)	0.600	(0.012)	443	0.237
nonafluoropentanoic acid	264.046	545.6	(0.5)	2.23	(0.05)	0.496	(0.01)	532	0.262
1,1,1,5,5,5-hexafluoro-2,4-pentanedione	208.059	485.1	(0.1)	2.77	(0.01)	0.72	(0.05)	289	0.198
1,1,1,2,4,4,4-heptafluoro-2-(trifluoromethoxy)butane	268.053	447.40	(0.05)	2.140	(0.005)	0.582	(0.005)	461	0.265
1,1,1,2,2,3,3-heptafluoropentan-4-one	212.066	476.55	(0.05)	2.578	(0.005)	0.538	(0.005)	394	0.256
3,4,4,4-tetrafluoro-3-(trifluoromethyl)-2-butanone	212.066	467.64	(0.05)	2.522	(0.005)	0.518	(0.005)	409	0.266
1,1,1,2,3,3-hexafluoro-3-(2,2,2-trifluoroethoxy)propane	250.062	475.74	(0.05)	2.233	(0.010)	0.563	(0.005)	444	0.251
1,1,1,3,3,3-hexafluoro-2-trifluoromethyl-2-(methoxy)propane	250.062	462.72	(0.05)	2.366	(0.005)	0.558	(0.005)	448	0.276
2,2,3,3,4,4,5,5,5-nonafluoro-1-pentanol	250.062	521.4	(1.0)	2.31	(0.10)	0.560	(0.011)	447	0.238
1,1,1,2,2-pentafluoro-3-(1,1,2,2-tetrafluoroethoxy)propane	250.062	473.01	(0.10)	2.244	(0.005)	0.550	(0.005)	455	0.259
2,2,3,3,4,4,5,5-octafluoro-1-pentanol	232.072	571.2	(1.0)	2.75	(0.10)	0.547	(0.011)	424	0.246
1,1,2,2-tetrafluoro-3-(1,1,2,2-tetrafluoroethoxy)propane	232.072	510.07	(0.05)	2.581	(0.005)	0.530	(0.005)	438	0.266
1,1,1,2,2-pentafluoropentan-3-one	176.085	475.54	(0.05)	2.642	(0.005)	0.494	(0.005)	356	0.238
4-methoxy-1,1,1,2,2,3,3-heptafluorobutane	214.081	481.54	(0.10)	2.381	(0.010)	0.497	(0.005)	431	0.256
pentafluorophenol	184.064	609	(5)	4.0	(0.1)	0.529	(0.005)	348	0.275
1,1,1,2,2,3,3,4,4-nonafluorohexan-5-one	262.073	498.97	(0.05)	2.198	(0.005)	0.520	(0.005)	504	0.267
1,1,1,2,3,3-hexafluoro-3-(2,2,3,3,3-pentafluoropropoxy)propane	300.070	486.48	(0.05)	1.950	(0.005)	0.567	(0.005)	529	0.255
2,2,3,3,4,4,5,5-octafluoropentanoic acid methyl ester	260.082	559.0	(0.5)	2.32	(0.05)	0.518	(0.01)	502	0.251
1,1,1,2,3,3-hexafluoro-3-(2,2,3,3-tetrafluoropropoxy)propane	282.079	507.6	(0.2)	1.84	(0.05)	0.533	(0.011)	529	0.231
4-ethoxy-1,1,1,2,2,3,3,4,4-nonafluorobutane	264.089	482.02	(0.10)	1.976	(0.005)	0.518	(0.005)	510	0.251
tridecafluoroheptanoyl chloride	382.507	519.8	(0.5)	1.45	(0.20)	0.587	(0.012)	652	0.219
2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoro-1-heptanol	350.077	554.7	(1.0)	2.35	(0.20)	0.577	(0.012)	607	0.309
2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-1-heptanol	332.087	589	(5)	2.03	(0.50)	0.552	(0.011)	602	0.249
1,1,2,2,3,3,4,4-octafluoro-5-(1,1,2,2-tetrafluoroethoxy)pentane	332.087	546.8	(1.0)	2.01	(0.05)	0.554	(0.011)	599	0.265
3,3,4,4,5,5,6,6-octafluoro-2-methyl-2-hexanol	260.125	589.4	(2.0)	2.43	(0.10)	0.488	(0.010)	533	0.264
1,1,5-trichloro-2,2,3,3,4,4,5,5-octafluoro-1-(1,1,1,2,3,3-hexafluoro-2-chloropropoxy)pentane	519.875	612.2	(2.0)	1.50	(0.05)	0.584	(0.012)	890	0.262
2,2,3,3,4,4,5-heptafluoro-5-(nonafluorobutyl)tetrahydrofuran	416.059	500.2	(0.2)	1.607	(0.020)	0.588	(0.006)	708	0.273
1-[1-[difluoro(pentafluoroethoxy)methyl]-1,2,2,2-tetrafluoroethoxy]-1,1,2,2,3,3,3-heptafluoropropane	470.056	481	(7)	1.35	(0.10)				
1,1,2,2-tetrafluoroethoxybenzene	194.126	603.8	(0.5)	2.85	(0.05)	0.426	(0.009)	456	0.259
2,4,6,8-tetraoxaheptadecafluorononanoic acid	528.073	551.2	(2.0)	0.73	(0.05)	0.513	(0.010)	1029	0.164
2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptanoic acid ethyl ester	374.124	575.6	(1.0)	1.27	(0.05)	0.496	(0.010)	754	0.200

Table 1 Continued

	molar mass M	T_c		p_c		ρ_c		V_c	
	g·mol^{-1}[a]	K[b]	(±)	MPa	(±)	g·cm^{-3}	(±)	cm^3·mol^{-1}	Z_c[c]
Halogens + O + S									
octafluoro-1,4-butanedisulfonyl difluoride	398.153	549.0	(1.0)	1.77	(0.05)	0.604	(0.012)	659	0.256
Halogens + S									
pentafluoro(trifluoromethyl)sulfur	196.063	381.2	(0.5)	3.37	(0.05)	0.69	(0.01)	284	0.302
thio-bis-trifluoromethane	170.077	376.8	(0.5)						
Halogens + Si									
trichloromethylsilane	149.479	517.5	(0.5)	3.53	(0.05)	0.435	(0.010)	344	0.282
trichloroethylsilane	163.506	560.0	(1.0)	3.33	(0.05)	0.406	(0.010)	403	0.288
dichlorodimethylsilane	129.061	520.4	(0.5)	3.49	(0.05)	0.369	(0.010)	350	0.282
chlorotrimethylsilane	108.642	497.8	(0.5)	3.20	(0.05)	0.297	(0.010)	366	0.283
dichlorodiethylsilane	157.114	595.8	(1.0)	3.06	(0.05)	0.345	(0.010)	455	0.281
N + O									
nitromethane	61.040	588	(2)	6.1	(0.3)	0.352	(0.010)	173	0.216
2-aminoethanol	61.083	675	(5)	7.6	(0.5)				
1,3-oxazole	69.062	551	(2)	6.77	(0.20)				
N,N-dimethylformamide	73.094	649.6	(0.5)			0.279	(0.005)	262	
N-methylacetamide	73.094	707.4	(1.0)	5.09	(0.10)				
2-(2-aminoethoxy)-ethanol	105.136	721	(2)	4.80	(0.10)				
2,2′-imino-bis-ethanol	105.136	737	(10)	4.3	(0.5)				
2-[(2-aminoethyl)amino]ethanol	104.151	739	(2)	4.65	(0.10)				
1-methyl-2-pyrrolidinone	99.131	721.8	(0.5)	4.52	(0.05)	0.319	(0.005)	311	0.234
4-formylmorpholine	115.130	779	(2)	5.08	(0.10)				
3-methyl-1-nitrosooxybutane	117.146	476.8	(0.5)	5.07	(0.05)				
N-methyldiethanolamine	119.162	742	(2)	4.16	(0.10)				
2,2′,2″-nitrilo-tris-ethanol	149.188	772	(10)	2.7	(0.5)				
isocyanatobenzene	119.121	657	(5)	4.00	(0.20)				
cyclohexyl-2-pyrrolidinone	167.248	810	(5)	2.2	(0.5)				
O + S									
sulfinyl-bis-methane	78.133					0.366	(0.010)	213	
ethanethioic acid *S*-ethyl ester	104.171	590.6	(0.2)	4.08	(0.1)	0.327	(0.006)	319	0.265
O + Si									
silicic acid tetramethyl ester	152.221	563.0	(0.5)	2.88	(0.05)				
hexamethyldisiloxane	162.378	518	(1)	1.92	(0.01)	0.275	(0.010)	590	0.263
hexamethylcyclotrisiloxane	222.462	554	(1)	1.79	(0.02)	0.315	(0.010)	706	0.274
1,1,1,3,5,5,5-heptamethyltrisiloxane	222.505	553.4	(0.2)	1.48	(0.02)				
silicic acid tetraethyl ester	208.328	592.2	(0.5)	2.05	(0.05)				
octamethyltrisiloxane	236.531	564	(1)	1.42	(0.01)	0.270	(0.010)	876	0.265
octamethylcyclotetrasiloxane	296.616	586.6	(1.0)	1.33	(0.05)	0.305	(0.010)	973	0.265
decamethyltetrasiloxane	310.685	599	(1)	1.19	(0.05)	0.270	(0.010)	1151	0.275
methyl-tris(trimethylsiloxy)silane	310.685	597	(1)	1.18	(0.05)	0.276	(0.010)	1126	0.268
decamethylcyclopentasiloxane	370.770	618	(2)	1.10	(0.10)	0.30	(0.01)	1236	0.265
silicic acid tetrapropyl ester	264.434	648	(1)	1.5	(0.2)				
hexaethyldisiloxane	246.537	693	(2)						
dodecamethylpentasiloxane	384.839	628	(1)	0.97	(0.05)	0.275	(0.010)	1399	0.260
tetrakis(trimethylsiloxy)silane	384.839	623	(1)	1.0	(0.1)	0.275	(0.010)	1399	0.270
tetradecamethylhexasiloxane	458.993	652	(2)	0.84	(0.05)	0.254	(0.010)	1807	0.280
tetradecamethylcycloheptasiloxane	519.078	684	(2)						
1,1,3,3-tetramethyl-1,3-diphenyldisiloxane	286.516	750	(8)	1.73	(0.03)				
silicic acid tetrabutyl ester	320.540	682	(7)	1.10	(0.03)				
hexadecamethylheptasiloxane	533.147	671.5	(1.0)	0.70	(0.10)	0.260	(0.010)	2051	0.257
octadecamethyloctasiloxane	607.301	689	(1)	0.68	(0.05)	0.260	(0.010)	2336	0.277
silicic acid tetrapentyl ester	376.646	714	(7)	0.89	(0.03)				
eicosamethylnonasiloxane	681.455	698.5	(1.0)	0.57	(0.05)	0.270	(0.010)	2524	0.248
(2α,4α,6α)-2,4,6-trimethyl-2,4,6-triphenylcyclotrisiloxane	408.670	824	(8)	1.34	(0.03)				
(2α,4α,6β)-2,4,6-trimethyl-2,4,6-triphenylcyclotrisiloxane	408.670	839	(8)	1.29	(0.03)				
docosamethyldecasiloxane	755.609	709.2	(0.5)	0.47	(0.05)				
silicic acid tetrahexyl ester	432.753	757	(8)	0.79	(0.02)				
1,3-dimethyl-1,1,3,3-tetraphenyldisiloxane	410.655	893	(9)	1.38	(0.03)				
silicic acid tetraheptyl ester	488.859	778	(8)	0.74	(0.02)				
silicic acid tetraoctyl ester	544.965	812	(8)	0.66	(0.02)				
silicic acid tetranonyl ester	601.072	830	(8)	0.61	(0.02)				
silicic acid tetradecyl ester	657.178	849	(8)	0.60	(0.02)				

[a] Molar masses are based on the following relative atomic masses: carbon, 12.010 7; hydrogen, 1.007 94; boron, 10.811; chlorine, 35.453; fluorine, 18.998 403 2; nitrogen, 14.006 7; oxygen, 15.999 4; sulfur, 32.065; silicon, 28.085 5 from *Pure Appl. Chem.* **2006**, *78*, 2051−2066. [b] Temperatures are expressed in ITS-90. [c] $Z_c = p_c V_c / RT_c$, where $R = 8.314\,472$ J·mol^{-1}·K^{-1}.

What Should Be Included in Table 2?

The criteria used to determine which values should be included have been discussed in the earlier parts, especially in part 1, but it was decided to offer here some clarifications, especially for the methods used to determine the critical properties (Table 4). All values are experimentally supported, directly measured for preference but in some cases obtained indirectly. They are important in themselves but are also important because they provide the basis for developing methods of calculating critical properties of substances for which there are no experimental values, necessary for the application of the principle of corresponding states, and for those to be valid, it is essential that they are based on experimental and not empirically estimated values.

The values included in Table 2 are based on experimental measurements made on pure samples of the compound inves-

Table 2. Critical Properties from the Literature

ref	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
		B + O				
		BORIC ACID TRIMETHYL ESTER (methyl borate): Molar Mass 103.913 g; $C_3H_9BO_3$; CASRN 121-43-7				
59-hug/pit[a]	(229.5 ± 0.5) °C, 502 psi	502.6*	3.46*		?, 5	Hughes et al.
60-gri/gor[b]	(228.5 ± 0.5) °C, (35.4 ± 0.4) atm	501.6*	3.59*		3, 5	Griskey et al.
	recommended values	502 ± 1	3.5 ± 0.1			
		Halogen(s) + N				
		TRIFLUOROETHANENITRILE (trifluoroacetonitrile): Molar Mass 95.023 g; C_2F_3N; CASRN 353-85-5				
		$T_{90} - T_{68} = -0.009$ at 311.1 K				
72-mou/kay, 75-mou[c]	(524.75 ± 0.5) psi	311.10 ± 0.2	3.618	0.470	1a, 5, 7	Mousa et al., Mousa
		DIFLUORO-*N,N*-bis(TRIFLUOROMETHYL)METHANAMINE: Molar Mass 203.034 g; C_3HF_8N; CASRN 73563-15-2				
98-sak/yas		404.94 ± 0.03	2.727 ± 0.002	0.591 ± 0.001	2	Sako et al.
		N,N-bis(TRIFLUOROMETHYL)METHANAMINE: Molar Mass 167.053 g; $C_3H_3F_6N$; CASRN 85034-09-9				
98-sak/yas		415.76 ± 0.03	2.916 ± 0.002	0.536 ± 0.001	2	Sako et al.
		2,2-DIFLUORO-*N,N*-bis(TRIFLUOROMETHYL)ETHANAMINE: Molar Mass 217.061 g; $C_4H_3F_8N$; CASRN 176674-31-0				
2003-ota/yas		460.20 ± 0.04	2.642 ± 0.002	0.579 ± 0.001	2	Otake et al.
		N,N-bis(TRIFLUOROMETHYL)ETHANAMINE: Molar Mass 181.080 g; $C_4H_5F_6N$; CASRN 85034-08-8				
98-sak/yas		442.60 ± 0.03	2.622 ± 0.002	0.490 ± 0.001	2	Sako et al.
		1,1,2,2,3,3,3-HEPTAFLUORO-*N,N*-bis(HEPTAFLUOROPROPYL)-1-PROPANAMINE (perfluorotripropylamine): Molar Mass 521.069 g; $C_9F_{21}N$; CASRN 338-83-0				
96-mus/ima		523.78 ± 8	1.352 ± 0.02		1, 5	Mustafaev et al.
		1,1,2,2,3,3,4,4,4-NONAFLUORO-*N*-NONAFLUOROBUTYL-*N*-(TRIFLUOROMETHYL)-1-BUTANAMINE (pefluoromethyldibutylamine): Molar Mass 521.069 g; $C_9F_{21}N$; CASRN 514-03-4				
96-mus/ima		529.49 ± 8	1.3596 ± 0.02		1, 5	Mustafaev et al.
		2,2,3,3,4,4,4a,5,5,6,6,7,7,8,8,8a-HEXADECAFLUORODECAHYDRO-1-(PENTAFLUOROETHYL)QUINOLINE (perfluoro-1-ethyldecahydroquinoline): Molar Mass 545.091 g; $C_{11}F_{21}N$; CASRN 130539-68-3				
96-mus/ima		574.88 ± 9	1.605 ± 0.02		1, 5	Mustafaev et al.
		1,1,2,2,3,3,4,4,4-NONAFLUORO-*N,N*-bis(NONAFLUOROBUTYL)-1-BUTANAMINE (perfluorotributylamine): Molar Mass 671.092 g; $C_{12}F_{27}N$; CASRN 311-89-7				
		$T_{90} - T_{68} = -0.039$ at 565.5 K				
80-toc/you	11.4 atm	565.42*	1.16*		1	Toczylkin and Young
96-mus/ima		561.09 ± 8	1.101 ± 0.02		1, 5	Mustafaev et al.
	recommended values	565.4 ± 0.5	1.16 ± 0.05			
		Halogen(s) + O				
		TRICHLOROACETYL CHLORIDE: Molar Mass 181.833 g; C_2Cl_4O; CASRN 76-02-8				
72-sok/gol[d]	333 °C	606.2*		0.55*	?, 7	Sokolova et al.
94-ste/chi		604* ± 1	4.32	0.520* ± 0.026	4, 6, 7	Steele et al.
	recommended values	605 ± 2	4.3 ± 0.2	0.53 ± 0.05		
		TRIFLUOROETHANOIC ACID (trifluoroacetic acid): Molar Mass 114.023 g; $C_2HF_3O_2$; CASRN 76-05-1				
		$T_{90} - T_{48} = 0.010$ at 491.3 K				
67-zaw	218.13 °C, 32.15 atm, 0.204 L·mol^{-1}	491.29	3.258	0.559	1, 7	Zawisza
		DIFLUOROMETHOXYTRIFLUOROMETHANE: Molar Mass 136.021 g; C_2HF_5O; CASRN 3822-68-2				
91-wan/adc[e]		353.85 ± 0.1	3.326		1, 5	Wang et al.
92-sal/wan	192 cm^3·mol^{-1}	353.54	3.326	0.708	1, 5, 7	Salvi-Narkhede et al.
96-sch/car		354.49* ± 0.02		0.5787* ± 0.008	1, 7	Schmidt et al.

Table 2 Continued

ref	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
96-web/def[f]		(354.49)	3.3508*		5/6	Weber and Defibaugh
	recommended values	354.49 ± 0.05	3.351 ± 0.005	0.579 ± 0.010		
		OXY-bis(DIFLUOROMETHANE): Molar Mass 118.030 g; $C_2H_2F_4O$; CASRN 1691-17-4				
92-def/gil		420.25 ± 0.02	4.228 ± 0.076	0.529 ± 0.010	2, 6, 7	Defibaugh et al.
		2,2,2-TRIFLUOROETHANOL: Molar Mass 100.040 g; $C_2H_3F_3O$; CASRN 75-89-8				
		$T_{90} - T_{68} = -0.040$ at 498.5 K				
74-mil[g]		499.78	4.46	0.481	?	Miller
87-bie		499.25 ± 0.1			2	Bier
89-bae/klo[h]		(499.29)	4.8606 ± 0.0001	0.487* ± 0.012	5, 7	Baehr et al.
89-bie/tue, 90-bie/tue		498.53* ± 0.05	4.825* ± 0.006		2, 5	Bier et al.
93-sau/hol[i]		(499.29)	4.870	0.484*	6, 7	Sauermann et al.
95-sin/mik	(226.0 ± 0.5) °C	499.2	4.75 ± 0.20	0.480 ± 0.005	1, 6, 7	Sinitsyn et al.
	recommended values	498.5 ± 0.1	4.825 ± 0.010	0.485 ± 0.005		
		TRIFLUOROMETHOXYMETHANE: Molar Mass 100.040 g; $C_2H_3F_3O$; CASRN 421-14-7				
91-wan/adc[e]	228 cm^3·mol^{-1}	378.05 ± 0.1	3.680	0.439	1, 5, 7	Wang et al.
92-sal/wan	228 cm^3·mol^{-1}	378.02	3.588	0.439	1, 5, 7	Salvi-Narkhede et al.
2001-yos, 2003-kay		377.921*	3.631*	0.465*	1, 5	Yoshii, Kayukawa
2003-kay/has		(377.921)	3.635*		5	Kayukawa et al.
2004-uch/yas		377.92* ± 0.01	3.640* ± 0.0005	0.459* ± 0.001	2	Uchida et al.
	recommended values	377.92 ± 0.10	3.635 ± 0.010	0.462 ± 0.010		
		CHLOROPENTAFLUORO-2-PROPANONE: Molar Mass 182.477 g; C_3ClF_5O; CASRN 79-53-8				
64-mur	137.5 °C, 28.40 atm	410.6	2.878		1, 5	Murphy
		HEXAFLUOROOXETANE (hexafluorotrimethylene oxide): Molar Mass 166.022 g; C_3F_6O; CASRN 425-82-1				
91-wan/adc[e]	272 cm^3·mol^{-1}	361.85 ± 0.1	3.094*	0.610	1, 5, 7	Wang et al.
92-sal/wan	272 cm^3·mol^{-1}	361.85	3.030*	0.610	1, 5, 7	Salvi-Narkhede et al.
	recommended values	361.9 ± 0.5	3.06 ± 0.05	0.61 ± 0.01		
		HEXAFLUORO-2-PROPANONE (hexafluoroacetone): Molar Mass 166.022 g; C_3F_6O; CASRN 684-16-2				
		$T_{90} - T_{68} = -0.022$ at 357.2 K				
64-mur	84.1 °C, 28.04 atm	357.2*	2.841*		1, 5	Murphy
69-glo/zaw	84.04 °C, 28.00 atm, 0.288 L·mol^{-1}	357.19*	2.837*	0.576*	1, 7	Główka and Zawisza
72-mou/kay, 76-mou[j]	(410.75 ± 0.5) psi	357.12* ± 0.2	2.832*	0.505*	1a, 5, 7	Mousa et al., Mousa
	recommended values	357.2 ± 0.5	2.84 ± 0.05	0.54 ± 0.05		
		TRIFLUORO(TRIFLUOROMETHYL)OXIRANE (1,2-epoxy-1,1,2,3,3,3-hexafluoropropane): Molar Mass 166.022 g; C_3F_6O; CASRN 428-59-1				
95-sin/mik	(86.5 ± 0.1) °C	359.6	2.93 ± 0.01	0.570 ± 0.006	1, 6, 7	Sinitsyn et al.
		HEXAFLUORO-1,3-DIOXOLANE: Molar Mass 182.021 g; $C_3F_6O_2$; CASRN 21297-65-4				
92-sal/wan		368.07	2.709		1, 5	Salvi-Narkhede et al.
		PENTAFLUORO(TRIFLUOROMETHOXY)ETHANE: Molar Mass 204.019 g; C_3F_8O; CASRN 665-16-7				
98-bey/des	83.7 °C	356.8		0.640	1, 7	Beyerlein et al.
		DIFLUORO-bis(TRIFLUOROMETHOXY)METHANE: Molar Mass 220.018 g; $C_3F_8O_2$; CASRN 53772-78-4				
91-wan/adc[e], 92-sal/wan	363 cm^3·mol^{-1}	372.35 ± 0.1	2.333	0.606	1, 5, 7	Wang et al., Salvi-Narkhede et al.

Table 2 Continued

ref	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
		1,1,1,2-TETRAFLUORO-2-(TRIFLUOROMETHOXY)ETHANE: Molar Mass 186.028 g; C_3HF_7O; CASRN 2356-62-9				
94-sak/sat		376.46 ± 0.1	2.6103* ± 0.002		2	Sako et al.
98-sak/yas		377.26* ± 0.03	2.621* ± 0.002	0.580 ± 0.001	2	Sako et al.
	recommended values	377.26 ± 0.10	2.616 ± 0.010	0.580 ± 0.005		
		1,1,2,2-TETRAFLUORO-1-(TRIFLUOROMETHOXY)ETHANE: Molar Mass 186.028 g; C_3HF_7O; CASRN 2356-61-8				
91-wan/adc[e]	337 cm^3·mol^{-1}	387.75* ± 0.1	2.640*	0.552*	1, 5, 7	Wang et al.
92-sal/wan	337 cm^3·mol^{-1}	387.78*	2.606*[j-1]	0.552*	1, 5, 7	Salvi-Narkhede et al.
	recommended values	387.8 ± 0.2	2.62 ± 0.05	0.55 ± 0.01		
		2-CHLORO-1-(DIFLUOROMETHOXY)-1,1,2-TRIFLUOROETHANE (enflurane): Molar Mass 184.492 g; $C_3H_2ClF_5O$; CASRN 13838-16-9				
		$T_{90} - T_{68} = -0.040$ at 475 K				
88-amb/ghi		474.99 ± 0.02	2.980 ± 0.005		1	Ambrose and Ghiassee
		2-CHLORO-2-(DIFLUOROMETHOXY)-1,1,1-TRIFLUOROETHANE (isoflurane): Molar Mass 184.492 g; $C_3H_2ClF_5O$; CASRN 26675-46-7				
		$T_{90} - T_{68} = -0.040$ at 468 K				
88-amb/ghi		467.76 ± 0.02	3.046 ± 0.005		1	Ambrose and Ghiassee
		1,1,1-TRIFLUORO-2-(TRIFLUOROMETHOXY)ETHANE: Molar Mass 168.038 g; $C_3H_2F_6$; CASRN 20193-67-3				
94-sak/sat		401.90 ± 0.1	2.8558 ± 0.002		2	Sako et al.
		1,1,1,2-TETRAFLUORO-2-(DIFLUOROMETHOXY)ETHANE: Molar Mass 168.038 g; $C_3H_2F_6O$; CASRN 57041-67-5				
94-sak/sat		428.82* ± 0.1	3.0341* ± 0.002		2	Sako et al.
96-sak/sat		428.95* ± 0.03	3.050* ± 0.002	0.533 ± 0.001	2	Sako et al.
	recommended values	428.90 ± 0.10	3.042 ± 0.010	0.533 ± 0.005		
		1,1,1-TRIFLUORO-2-(DIFLUOROMETHOXY)ETHANE: Molar Mass 150.047 g; $C_3H_3F_5O$; CASRN 1885-48-9				
94-sch[k]		443.992 ± 0.02			4	Schmidt
98-goo/def[l]		(443.992)	3.048 ± 0.062		5/6	Goodwin et al.
		1,2,2-TRIFLUORO-2-(DIFLUOROMETHOXY)ETHANE: Molar Mass 150.047 g; $C_3H_3F_5O$;CASRN 69948-24-9				
98-sak/yas		462.03 ± 0.03	3.538 ± 0.002	0.533 ± 0.001	2	Sako et al.
		PENTAFLUORO(METHOXY)ETHANE: Molar Mass 150.047 g; $C_3H_3F_5O$; CASRN 22410-44-2				
94-sak/sat		406.74 ± 0.1	2.8720 ± 0.002		2	Sako et al.
96-sak/sat		406.80* ± 0.03	2.887* ± 0.002	0.499* ± 0.001	2	Sako et al.
98-tsu/sat		(406.80)	2.8863* ± 0.0015		5	Tsuge et al.
2001-yos/miz		406.830* ± 0.017		0.509* ± 0.003	2	Yoshii et al.
2003-kay/has		(406.83)	2.887*		5	Kayukawa et al.
2004-ota/uch		406.82* ± 0.01	2.885* ± 0.0005	0.491* ± 0.001	2	Otake et al.
	recommended values	406.82 ± 0.05	2.886 ± 0.005	0.500 ± 0.010		
		2,2,3,3-TETRAFLUORO-1-PROPANOL: Molar Mass 132.057 g; $C_3H_4F_4O$; CASRN 76-37-9				
95-sin/mik	(280.5 ± 0.7) °C	553.6	4.63 ± 0.05	0.496 ± 0.005	1, 6, 7	Sinitsyn et al.
		CARBONCHLORIDIC ACID ETHYL ESTER (ethyl chloroformate): Molar Mass 108.524 g; $C_3H_5ClO_2$; CASRN 541-41-3				
02-guy/mal	<235 °C	<508			1	Guye and Mallet
		1,1,1-TRIFLUORO-2-(METHOXY)ETHANE: Molar Mass 114.066 g; $C_3H_5F_3O$; CASRN 460-43-5				
94-sak/sat		449.15* ± 0.1	3.5041* ± 0.002		2	Sako et al.
96-sak/sat		448.98* ± 0.03	3.513* ± 0.002	0.412 ± 0.001	2	Sako et al.
	recommended values	449.05 ± 0.10	3.509 ± 0.010	0.412 ± 0.005		
		OCTAFLUOROTETRAHYDROFURAN: Molar Mass 216.029 g; C_4F_8O; CASRN 773-14-8				
93-sal/adc	318 cm^3·mol^{-1}	399.96	2.694	0.679	1, 5, 7	Salvi-Narkhede et al.

Table 2 Continued

ref	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
		1,1,1,2,2,3,3-HEPTAFLUORO-3-(TRIFLUOROMETHOXY)PROPANE: Molar Mass 254.026 g; $C_4F_{10}O$; CASRN 59426-77-6				
93-sal/adc	403 cm^3·mol^{-1}	391.7	1.866	0.630	1, 5, 7	Salvi-Narkhede et al.
		2,2,3,3,5,5,6-HEPTAFLUORO-1,4-DIOXANE: Molar Mass 214.038 g; $C_4HF_7O_2$; CASRN 34118-18-8				
2001-sak/yas		452.88 ± 0.03	2.866 ± 0.002	0.597 ± 0.001	2	Sako et al.
		4,4,5,5-TETRAFLUORO-2-(TRIFLUOROMETHYL)-1,3-DIOXOLANE: Molar Mass 214.038 g; $C_4HF_7O_2$; CASRN 269716-57-6				
2001-sak/yas		435.06 ± 0.03	2.645 ± 0.002	0.569 ± 0.001	2	Sako et al.
		PENTAFLUORO(1,1,2,2-TETRAFLUOROETHOXY)ETHANE: Molar Mass 236.036 g; C_4HF_9O; CASRN 134769-21-4				
98-sak/yas		412.63 ± 0.03	2.257 ± 0.002	0.499 ± 0.001	2	Sako et al.
		PENTAFLUORO(2,2,2-TRIFLUOROETHOXY)ETHANE: Molar Mass 218.045 g; $C_4H_2F_8O$; CASRN 156053-88-2				
94-sak/sat		421.50* ± 0.1	2.3243* ± 0.002		2	Sako et al.
96-sak/sat		421.68* ± 0.03	2.330* ± 0.002	0.533 ± 0.001	2	Sako et al.
	recommended values	421.60 ± 0.10	2.327 ± 0.010	0.533 ± 0.005		
		1,1,1,3,3,3-HEXAFLUORO-2-(DIFLUOROMETHOXY)PROPANE: Molar Mass 218.045 g; $C_4H_2F_8O$; CASRN 26103-08-2				
98-sak/yas		444.63 ± 0.03	2.571 ± 0.002	0.581 ± 0.001	2	Sako et al.
		1,1-bis(DIFLUOROMETHOXY)-1,2,2,2-TETRAFLUOROETHANE: Molar Mass 234.045 g; $C_4H_2F_8O_2$; CASRN 267901-02-0				
2001-sak/yas		449.81 ± 0.03	2.421 ± 0.002	0.571 ± 0.001	2	Sako et al.
		3,3,4,4,4-PENTAFLUORO-2-BUTANONE: Molar Mass 162.058 g; $C_4H_3F_5O$; CASRN 374-41-4				
2001-sak/yas		453.03 ± 0.03	2.912 ± 0.002	0.486 ± 0.001	2	Sako et al.
		3-DIFLUOROMETHOXY-1,1,1,2,2-PENTAFLUOROPROPANE: Molar Mass 200.055 g; $C_4H_3F_7O$; CASRN 56860-81-2				
2003-yas/yam		455.10 ± 0.04	2.773 ± 0.004	0.576 ± 0.001	2	Yasumoto et al.
		1,1,1,2,2,3,3-HEPTAFLUORO-3-(METHOXY)PROPANE: Molar Mass 200.055 g; $C_4H_3F_7O$; CASRN 375-03-1				
94-sak/sat		437.47* ± 0.1	2.4836* ± 0.002		2	Sako et al.
96-sak/sat		437.70* ± 0.03	2.481* ± 0.002	0.530 ± 0.001	2	Sako et al.
98-uch/wid		(437.70)	2.4759* ± 0.0017		5	Uchimura et al.
	recommended values	437.60 ± 0.10	2.480 ± 0.010	0.530 ± 0.005		
		1,1,1,2,3,3,3-HEPTAFLUORO-2-(METHOXY)PROPANE: Molar Mass 200.055 g; $C_4H_3F_7O$; CASRN 22052-84-2				
94-sak/sat		433.12* ± 0.1	2.5433* ± 0.002		2	Sako et al.
96-sak/sat		433.30* ± 0.03	2.553* ± 0.002	0.542 ± 0.001	2	Sako et al.
	recommended values	433.21* ± 0.10	2.548* ± 0.010	0.542 ± 0.005		
		1,1,2,2-TETRAFLUORO-1-(2,2,2-TRIFLUOROETHOXY)ETHANE: Molar Mass 200.055 g; $C_4H_3F_7O$; CASRN 406-78-0				
2003-yas/yam		463.89 ± 0.02	2.713 ± 0.001	0.541 ± 0.001	2	Yasumoto et al.
		1,1,1,3,3,3-HEXAFLUORO-2-(METHOXY)PROPANE: Molar Mass 182.064 g; $C_4H_4F_6O$; CASRN 13171-18-1				
94-sak/sat		459.61* ± 0.1	2.6929* ± 0.002		2	Sako et al.
98-sak/yas		459.58* ± 0.03	2.699* ± 0.002	0.481 ± 0.001	2	Sako et al.
	recommended values	459.60 ± 0.10	2.696 ± 0.010	0.481 ± 0.005		
		1,1,2,2-TETRAFLUORO-2-(2,2-DIFLUOROETHOXY)ETHANE: Molar Mass 182.064 g; $C_4H_4F_6O$; CASRN 50807-77-7				
2003-yas/yam		501.08 ± 0.02	3.090 ± 0.004	0.520 ± 0.001	2	Yasumoto et al.
		1,1,1-TRIFLUORO-2-(2,2,2-TRIFLUOROETHOXY)ETHANE: Molar Mass 182.064 g; $C_4H_4F_6O$; CASRN 333-36-8				
2003-yas/yam		476.31 ± 0.03	2.783 ± 0.002	0.500 ± 0.001	2	Yasumoto et al.

Table 2 Continued

ref	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
		PENTAFLUORO(ETHOXY)ETHANE: Molar Mass 164.074 g; $C_4H_5F_5O$; CASRN 22052-81-9				
94-sak/sat		431.03* ± 0.1	2.5187* ± 0.002		2	Sako et al.
96-sak/sat		431.23* ± 0.03	2.533* ± 0.002	0.448 ± 0.001	2	Sako et al.
	recommended values	431.13 ± 0.10	2.526 ± 0.010	0.448 ± 0.005		
		3-METHOXY-1,1,2,2-TETRAFLUOROPROPANE: Molar Mass 146.083 g; $C_4H_6F_4O$; CASRN 60598-17-6				
2003-yas/yam		505.35 ± 0.02	3.279 ± 0.002	0.453 ± 0.001	2	Yasumoto et al.
		NONAFLUOROPENTANOYL FLUORIDE: Molar Mass 266.037 g; $C_5F_{10}O$; CASRN 375-62-2				
95-sin/mik	(154.0 ± 3.0) °C	427	1.90 ± 0.09	0.600 ± 0.006	1, 6, 7	Sinitsyn et al.
		NONAFLUOROPENTANOIC ACID: Molar Mass 264.046 g; $C_5HF_9O_2$; CASRN 2706-90-3				
95-sin/mik	(272.4 ± 0.2) °C	545.6	2.23 ± 0.03	0.553 ± 0.006	1, 6, 7	Sinitsyn et al.
		1,1,1,5,5,5-HEXAFLUORO-2,4-PENTANEDIONE (hexafluoroacetylacetone): Molar Mass 208.059 g; $C_5H_2F_6O_2$; CASRN 1522-22-1				
		$T_{90} - T_{68} = -0.040$ at 485.1 K				
81-mou	1.39 cm^3·g^{-1}	485.06 ± 0.02	2.76716 ± 0.00069	0.719	1a, 5, 7	Mousa
		1,1,1,2,4,4,4-HEPTAFLUORO-2-(TRIFLUOROMETHOXY)BUTANE: Molar Mass 268.053 g; $C_5H_2F_{10}O$; CASRN 347148-74-7				
2001-sak/yas		447.40 ± 0.03	2.140 ± 0.002	0.582 ± 0.001	2	Sako et al.
		1,1,1,2,2,3,3-HEPTAFLUOROPENTAN-4-ONE: Molar Mass 212.066 g; $C_5H_3F_7O$; CASRN 355-17-9				
2003-ota/yas		476.55 ± 0.03	2.578 ± 0.001	0.538 ± 0.001	2	Otake et al.
		3,4,4,4-TETRAFLUORO-3-(TRIFLUOROMETHYL)-2-BUTANONE: Molar Mass 212.066 g; $C_5H_3F_7O$; CASRN 80553-01-1				
2001-sak/yas		467.64 ± 0.03	2.522 ± 0.002	0.518 ± 0.001	2	Sako et al.
		1,1,1,2,3,3-HEXAFLUORO-3-(2,2,2-TRIFLUOROETHOXY)PROPANE: Molar Mass 250.062 g; $C_5H_3F_9O$; CASRN 993-95-3				
2003-yas/yam		475.74 ± 0.03	2.233 ± 0.005	0.563 ± 0.001	2	Yasumoto et al.
		1,1,1,3,3,3-HEXAFLUORO-2-TRIFLUOROMETHYL-2-(METHOXY)PROPANE (*tert*-perfluorobutyl methyl ether): Molar Mass 250.062 g; $C_5H_3F_9O$; CASRN 66670-22-2				
2001-sak/yas		462.72 ± 0.03	2.366 ± 0.002	0.558 ± 0.001	2	Sako et al.
		2,2,3,3,4,4,5,5,5-NONAFLUORO-1-PENTANOL: Molar Mass 250.062 g; $C_5H_3F_9O$; CASRN 355-28-2				
95-sin/mik	(248.3 ± 0.5) °C	521.4	2.31 ± 0.02	0.560 ± 0.006	1, 6, 7	Sinitsyn et al.
		1,1,1,2,2-PENTAFLUORO-3-(1,1,2,2-TETRAFLUOROETHOXY)PROPANE; Molar Mass 250.062 g; $C_5H_3F_9O$; CASRN 50807-74-4				
2003-yas/yam		473.01 ± 0.04	2.244 ± 0.002	0.550 ± 0.001	2	Yasumoto et al.
		2,2,3,3,4,4,5,5-OCTAFLUORO-1-PENTANOL: Molar Mass 232.072 g; $C_5H_4F_8O$; CASRN 355-80-6				
95-sin/mik	(298.0 ± 0.5) °C	571.2	2.75 ± 0.05	0.547 ± 0.006	1, 6, 7	Sinitsyn et al.
		1,1,2,2-TETRAFLUORO-3-(1,1,2,2-TETRAFLUOROETHOXY)PROPANE: Molar Mass 232.072 g; $C_5H_4F_8O$; CASRN 16627-68-2				
2003-yas/yam		510.07 ± 0.02	2.581 ± 0.002	0.530 ± 0.001	2	Yasumoto et al.
		1,1,1,2,2-PENTAFLUOROPENTAN-3-ONE: Molar Mass 176.085 g; $C_5H_5F_5O$; CASRN 378-72-3				
2003-ota/yas		475.54 ± 0.03	2.642 ± 0.002	0.494 ± 0.001	2	Otake et al.
		4-METHOXY-1,1,1,2,2,3,3-HEPTAFLUOROBUTANE: Molar Mass 214.081 g; $C_5H_5F_7O$; CASRN 376-98-7				
2003-yas/yam		481.54 ± 0.07	2.381 ± 0.004	0.497 ± 0.001	2	Yasumoto et al.
		PENTAFLUOROPHENOL: Molar Mass 184.064 g; C_6HF_5O; CASRN 771-61-9				
71-amb/spr[m]		609 ± 5	4.0 ± 0.1		1	Ambrose and Sprake
74-hal/tow		(609)		0.529	7	Hales and Townsend

Table 2 Continued

ref	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
		1,1,1,2,2,3,3,4,4-NONAFLUOROHEXAN-5-ONE: Molar Mass 262.073 g; $C_6H_3F_9O$; CASRN 678-18-2				
2003-ota/yas		498.97 ± 0.03	2.198 ± 0.002	0.520 ± 0.001	2	Otake et al.
		1,1,1,2,3,3-HEXAFLUORO-3-(2,2,3,3,3-PENTAFLUOROPROPOXY)PROPANE: Molar Mass 300.070 g; $C_6H_3F_{11}O$; CASRN 1000-28-8				
2003-yas/yam		486.48 ± 0.02	1.950 ± 0.003	0.567 ± 0.001	2	Yasumoto et al.
		2,2,3,3,4,4,5,5-OCTAFLUOROPENTANOIC ACID METHYL ESTER: Molar Mass 260.082 g; $C_6H_4F_8O_2$; CASRN 54822-22-9				
95-sin/mik	(285.9 ± 0.2) °C	559.0	2.32 ± 0.03	0.518 ± 0.005	1, 6,7	Sinitsyn et al.
		1,1,1,2,3,3-HEXAFLUORO-3-(2,2,3,3-TETRAFLUOROPROPOXY)PROPANE: Molar Mass 282.079 g; $C_6H_4F_{10}O$; CASRN 65064-78-0				
95-sin/mik	(234.5 ± 0.1) °C	507.6	1.84 ± 0.02	0.533 ± 0.006	1, 6,7	Sinitsyn et al.
		4-ETHOXY-1,1,1,2,2,3,3,4,4-NONAFLUOROBUTANE[n]: Molar Mass 264.089 g; $C_6H_5F_9O$; CASRN 16370-05-4				
2003-yas/yam		482.02 ± 0.05	1.976 ± 0.002	0.518 ± 0.001	2	Yasumoto et al.
		TRIDECAFLUOROHEPTANOYL CHLORIDE: Molar Mass 382.507; $C_7ClF_{13}O$ g; CASRN 52447-22-0				
95-sin/mik	(246.6 ± 0.2) °C	519.8	1.45 ± 0.10	0.587 ± 0.006	1, 6,7	Sinitsyn et al.
		2,2,3,3,4,4,5,5,6,6,7,7,7-TRIDECAFLUORO-1-HEPTANOL: Molar Mass 350.077 g; $C_7H_3F_{13}O$; CASRN 375-82-6				
95-sin/mik	(281.5 ± 0.5) °C	554.7	2.35 ± 0.10	0.577 ± 0.006	1, 6,7	Sinitsyn et al.
		2,2,3,3,4,4,5,5,6,6,7,7-DODECAFLUORO-1-HEPTANOL: Molar Mass 332.087 g; $C_7H_4F_{12}O$; CASRN 355-99-9				
95-sin/mik	(316.0 ± 5.0) °C	589	2.03 ± 0.20	0.552 ± 0.006	1, 6,7	Sinitsyn et al.
		1,1,2,2,3,3,4,4-OCTAFLUORO-5-(1,1,2,2-TETRAFLUOROETHOXY)PENTANE: Molar Mass 332.087 g; $C_7H_4F_{12}O$; CASRN 16627-71-7				
95-sin/mik	(273.7 ± 0.5) °C	546.8	2.01 ± 0.02	0.554 ± 0.006	1, 6,7	Sinitsyn et al.
		3,3,4,4,5,5,6,6-OCTAFLUORO-2-METHYL-2-HEXANOL: Molar Mass 260.125 g; $C_7H_8F_8O$; CASRN 2673-15-6				
95-sin/mik	(316.2 ± 2.0) °C	589.4	2.43 ± 0.05	0.488 ± 0.005	1, 6,7	Sinitsyn et al.
		1,1,5-TRICHLORO-2,2,3,3,4,4,5,5-OCTAFLUORO-1-(1,1,1,2,3,3-HEXAFLUORO-2-CHLOROPROPOXY)PENTANE: Molar Mass 519.875 g; $C_8Cl_4F_{14}O$; CASRN 912670-61-2				
95-sin/mik	(339.0 ± 2.0) °C	612.2	1.50 ± 0.03	0.584 ± 0.006	1, 6,7	Sinitsyn et al.
		2,2,3,3,4,4,5-HEPTAFLUORO-5-(NONAFLUOROBUTYL)TETRAHYDROFURAN: Molar Mass 416.059 g; $C_8F_{16}O$; CASRN 335-36-4				
		$T_{90} - T_{48} = 0.013$ at 500.2 K				
57-thr[o], 60-yar/kay[p]	227.06 °C, 15.861 atm, 0.70738 L·mol^{-1}	500.22	1.6071	0.58817	1a,5,7	Throckmorton, Yarrington and Kay
		1-[1-[DIFLUORO(PENTAFLUOROETHOXY)METHYL]-1,2,2,2-TETRAFLUOROETHOXY]-1,1,2,2,3,3,3-HEPTAFLUOROETHANE (5-trifluoromethylperfluoro-3,6-dioxanonane): Molar Mass 470.056 g; $C_8F_{18}O_2$; CASRN 66804-94-2				
96mus/ima		480.91 ± 7	1.345 ± 0.02		1, 5	Mustafaev et al.
		1,1,2,2-TETRAFLUOROETHOXYBENZENE: Molar Mass 194.126 g; $C_8H_6F_4O$; CASRN 350-57-2				
95-sin/mik	(330.6 ± 0.2) °C	603.8	2.85 ± 0.02	0.426 ± 0.004	1, 6,7	Sinitsyn et al.
		2,4,6,8-TETRAOXAHEPTADECAFLUORONONANOIC ACID: Molar Mass 528.073 g; $C_9HF_{17}O_6$; CASRN 252556-93-7				
95-sin/mik[q]	(278.0 ± 2.0) °C	551.2	0.73 ± 0.03	0.513 ± 0.005	1, 6,7	Sinitsyn et al.
		2,2,3,3,4,4,5,5,6,6,7,7-DODECAFLUOROHEPTANOIC ACID ETHYL ESTER: Molar Mass 374.124 g; $C_9H_6F_{12}O_2$; CASRN 42287-85-4				
95-sin/mik	(302.5 ± 0.5) °C	575.6	1.27 ± 0.03	0.496 ± 0.005	1, 6,7	Sinitsyn et al.
		Halogen(s) + O + S				
		OCTAFLUORO-1,4-BUTANEDISULFONYL DIFLUORIDE: Molar Mass 398.153 g; $C_4F_{10}O_6S_2$; CASRN 84246-31-1				
95-sin/mik	(275.9 ± 0.5) °C	549.0	1.77 ± 0.02	0.604 ± 0.006	1, 6,7	Sinitsyn et al.
		Halogen(s) + S				
		PENTAFLUORO(TRIFLUOROMETHYL)SULFUR: Molar Mass 196.063 g; CF_8S; CASRN 373-80-8				
98-bey/des	108.1 °C	381.2	3.371	0.690	1, 6,7	Beyerlein et al.
		THIO-bis-TRIFLUOROMETHANE: Molar Mass 170.077 g; C_2F_6S; CASRN 371-78-8				
98-bey/des	103.6 °C	376.8			1	Beyerlein et al.
		Halogen(s) + Si				
		TRICHLOROMETHYLSILANE: Molar Mass 149.479 g; CH_3Cl_3Si; CASRN 75-79-6				
67-ste, 72-ste[r]	(244.6 ± 0.3) °C,	517.8*	3.53	0.440* ± 0.004	4, 5,7	Stepanov

Table 2 Continued

ref	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
	(34.8 ± 0.11) atm					
73-sok/pro[s]	244 °C	517.2*		0.43*	?, 7	Sokolova et al.
	recommended values	517.5 ± 0.5	3.53 ± 0.05	0.435 ± 0.010		
		TRICHLOROETHYLSILANE: Molar Mass 163.506 g; $C_2H_5Cl_3Si$; CASRN 115-21-9				
67-ste,	(286.8 ± 0.5) °C,	560.0	3.33	0.406 ± 0.004	4, 5,7	Stepanov,
68-ste/noz[r]	(32.9 ± 0.11) atm					Stepanov and Nozdrev
		DICHLORODIMETHYLSILANE: Molar Mass 129.061 g; $C_2H_6Cl_2Si$; CASRN 75-78-5				
67-ste,	(247.2 ± 0.3) °C,	520.4	3.49	0.369 ± 0.004	4, 5,7	Stepanov,
68-ste/noz[r]	(34.4 ± 0.11) atm					Stepanov and Nozdrev
		CHLOROTRIMETHYLSILANE: Molar Mass 108.642 g; C_3H_9ClSi; CASRN 75-77-4				
68-ste/noz[r]	(224.6 ± 0.3) °C, (31.6 ± 0.11) atm	497.8	3.20	0.297 ± 0.003	4, 5,7	Stepanov and Nozdrev
		DICHLORODIETHYLSILANE: Molar Mass 157.114 g; $C_4H_{10}Cl_2Si$; CASRN 1719-53-5				
72-ste	(322.6 ± 0.6) °C, (30.2 ± 0.11) atm	595.8	3.06	0.345 ± 0.003	4, 5,7	Stepanov
		N + O				
		NITROMETHANE: Molar Mass 61.040 g; CH_3NO_2; CASRN 75-52-5				
49-gri	(315 ± 1) °C, (915 ± 15) psi	588.2	6.31*	0.352 ± 0.004	3	Griffin
78-amb/cou		(588.2)	5.87*		6	Ambrose et al.
	recommended values	588 ± 2	6.1 ± 0.3	0.352 ± 0.010		
		2-AMINOETHANOL (ethanolamine): Molar Mass 61.083 g; C_2H_7NO; CASRN 141-43-5				
85-lyo	(405.0 ± 3.8) °C	678.2*	7.124* ± 0.328		1a, 6	Lyons
90-ans/tej[f]		>670*			1	Anselme and Teja
91-tej/ros[u]		671.4* ± 1.4	8.03* ± 0.04		2c	Teja and Rosenthal
	recommended values	675 ± 5	7.6 ± 0.5			
		1,3-OXAZOLE: Molar Mass 69.062 g; C_3H_3NO; CASRN 288-42-6				
2006-von/wil		550.8 ± 2	6.77 ± 0.14		3	VonNiederhausern et al.
		N,*N*-DIMETHYLFORMAMIDE: Molar Mass 73.094 g; C_3H_7NO; CASRN 68-12-2				
90-tej/ans		649.6 ± 0.4		0.279 ± 0.005	1	Teja and Anselme
		N-METHYLACETAMIDE: Molar Mass 73.094 g; C_3H_7NO; CASRN 79-16-3				
2004-von/gil		707.4 ± 1.0	5.09 ± 0.10		3	VonNiederhausern and Giles
		2-(2-AMINOETHOXY)ETHANOL: Molar Mass 105.136 g; $C_4H_{11}NO_2$; CASRN 929-06-6				
2006-von/wil		721.2 ± 2	4.80 ± 0.10		3	VonNiederhausern et al.
		2,2′-IMINO-bis-ETHANOL (diethanolamine): Molar Mass 105.136 g; $C_4H_{11}NO_2$; CASRN 111-42-2				
85-lyo	(463.4 ± 8.1) °C	736.6	4.270 ± 0.453		1a, 6	Lyons
		2-[(2-AMINOETHYL)AMINO]ETHANOL: Molar Mass 104.151 g; $C_4H_{12}N_2O$; CASRN 111-41-1				
2002-wil/von		739.2 ± 2	4.65 ± 0.10		3	Wilson et al.
		1-METHYL-2-PYRROLIDINONE (*N*-methyl pyrrolidone): Molar Mass 99.131 g; C_5H_9NO; CASRN 872-50-4				
90-tej/ans-1		721.8* ± 0.3		0.319 ± 0.005	1	Teja and Anselme
94-gud/tej		721.7* ± 0.4	4.52 ± 0.02		2c	Gude and Teja
	recommended values	721.8 ± 0.5	4.52 ± 0.05	0.319 ± 0.005		
		4-FORMYLMORPHOLINE: Molar Mass 115.130 g; $C_5H_9NO_2$; CASRN 4394-85-8				
2006-von/wil		779.3 ± 2	5.08 ± 0.10		3	VonNiederhausern et al.
		3-METHYL-1-NITROSOOXYBUTANE (isopentyl nitrite [ester]): Molar Mass 117.146 g; $C_5H_{11}NO_2$; CASRN 110-46-3				
2000-lia/ma		476.81	5.07		1	Liang et al.
		N-METHYLDIETHANOLAMINE: Molar Mass 119.162 g; $C_5H_{13}NO_2$; CASRN 105-59-9				
2006-von/wil		741.9 ± 2	4.16 ± 0.08		3	VonNiederhausern et al.
		2,2′,2″-NITRILO-tris-ETHANOL (triethanolamine): Molar Mass 149.188 g; $C_6H_{15}NO_3$; CASRN 102-71-6				
85-lyo	(498.9 ± 9.8) °C	772.0	2.743 ± 0.438		1a, 6	Lyons
		ISOCYANATOBENZENE (phenyl isocyanate)[v]: Molar Mass 119.121 g; C_7H_5NO; CASRN 103-71-9				
2006-von/wil		656.9 ± 5	4.00 ± 0.20		3	VonNiederhausern et al.
		1-CYCLOHEXYL-2-PYRROLIDINONE (*N*-cyclohexyl pyrrolidone): Molar Mass 167.248 g; $C_{10}H_{17}NO$; CASRN 6837-24-7				
85-lyo	(537.2 ± 4.0) °C	810.4	2.172 ± 0.213		1a, 6	Lyons

Table 2 Continued

ref	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
		O + S				
		SULFINYL-bis-METHANE (methyl sulfoxide): Molar Mass 78.133 g; C_2H_6OS; CASRN 67-68-5				
79-cam[w]				0.366	7	Campbell
		ETHANETHIOIC ACID S-ETHYL ESTER (ethyl thioacetate): Molar Mass 104.171 g; C_4H_8OS; CASRN 625-60-5				
96-wil/wil		590.55 ± 0.1	4.075 ± 0.069	0.327 ± 0.006	1a	Wilson et al.
		O + Si				
		SILICIC ACID TETRAMETHYL ESTER (tetramethoxysilane): Molar Mass 152.221 g; $C_4H_{12}O_4Si$; CASRN 681-84-5				
78-wat/you[x]	(28.35 ± 0.07) atm	562.8* ± 0.2	2.873*		1	Waterson and Young
2008-nik/pop		558 ± 6	2.89* ± 0.09		4	Nikitin et al.
	recommended values	563.0 ± 0.5	2.88 ± 0.05			
		HEXAMETHYLDISILOXANE (MM): Molar Mass 162.378 g; $C_6H_{18}OSi_2$; CASRN 107-46-0				
57-pol	245.3 °C, 611 cm^3·mol^{-1}	518.4*		0.266*	1, 7	Pollnow
72-you-1,-2[y]	18.85 atm	516.6* ± 0.2	1.910*		1	Young
74-dic/mcl[z]		518.8* ± 0.2	1.91* ± 0.02		1	Dickinson and McLure
76-mcl/dic		(518.7)	1.925* ± 0.01		5	McLure and Dickinson
77-mcl/nev[aa]		(516.6)		0.258 ± 0.005	7	McLure and Neville
86-ale	573 cm^3·mol^{-1}	516.6*	1.905*	0.283*	3	Aleksandrova
86-fla		(518.7)	1.939		6	Flaningam
94-nik/pav		519* ± 5	1.92* ± 0.04		4	Nikitin et al.
	recommended values	518 ± 1	1.92 ± 0.01	0.275 ± 0.010		
		HEXAMETHYLCYCLOTRISILOXANE (D_3): Molar Mass 222.462 g; $C_6H_{18}O_3Si_3$; CASRN 541-05-9				
57-pol	281.0 °C, 707 cm^3·mol^{-1}	554.2		0.315	1, 7	Pollnow
86-fla		(554.2)	1.788		6	Flaningam
		1,1,1,3,5,5,5-HEPTAMETHYLTRISILOXANE: Molar Mass 222.505 g; $C_7H_{22}O_2Si_3$; CASRN 1873-88-7				
79-mye/her		553.40	1.481		1a	Myers et al.
		SILICIC ACID TETRAETHYL ESTER (tetraethoxysilane): Molar Mass 208.328 g; $C_8H_{20}O_4Si$; CASRN 78-10-4				
32-sol/mol		611			1	Solana and Moles
78-wat/you[x]	(20.18 ± 0.07) atm	592.2* ± 0.2	2.045*		1	Waterson and Young
2008-nik/pop		587 ± 6	2.04* ± 0.06		4	Nikitin et al.
	recommended values	592.2 ± 0.5	2.05 ± 0.05			
		OCTAMETHYLTRISILOXANE (MDM): Molar Mass 236.531 g; $C_8H_{24}O_2Si_3$; CASRN 107-51-7				
57-pol	291.2 °C, 868 cm^3 ·mol^{-1}	564.4*		0.2725*	1, 7	Pollnow
72-you-2[y]	14.01 atm	562.9*	1.420*		1	Young
74-dic/mcl[z]		565.4* ± 0.2	1.46 ± 0.02		1	Dickinson and McLure
77-mcl/nev[aa]		(562.9)		0.261 ± 0.005	7	McLure and Neville
86-fla		(564.4)	1.440		6	Flaningam
90-lin/her		564.13* ± 0.10	1.415* ± 0.007	0.2683*	1a, 5, 7	Lindley and Hershey
	recommended values	564 ± 1	1.42 ± 0.01	0.270 ± 0.010		
		OCTAMETHYLCYCLOTETRASILOXANE (D_4): Molar Mass 296.616 g; $C_8H_{24}O_4Si_4$; CASRN 556-67-2				
54-ost/gru[bb]		587* ± 2		0.31*	1, 7	Osthoff and Grubb
57-pol	314.2 °C, 970 cm^3·mol^{-1}	587.4*		0.306*	1, 7	Pollnow
71-hic/you[cc]	13.07 atm	586.5*	1.324*		1	Hicks and Young
72-you	(13.66 ± 0.07) kg·cm^{-2}, (984 ± 3) cm^3·mol^{-1}	586.5* ± 0.2	1.340*	0.301*	1, 7	Young
82-mcl/nev[dd]		585.7* ± 0.3	1.32* ± 0.02	0.295 ± 0.006	1, 7	McLure and Neville
86-fla		(586.8)	1.344		6	Flaningam
	recommended values	586.6 ± 1.0	1.33 ± 0.05	0.305 ± 0.010		
		DECAMETHYLTETRASILOXANE (MD_2M): Molar Mass 310.685 g; $C_{10}H_{30}O_3Si_4$; CASRN 141-62-8				
57-pol	326.0 °C, 1157 cm^3 ·mol^{-1}	599.2*		0.2685*	1, 7	Pollnow
72-you-2[y]	12.48 atm	599.4*	1.265		1	Young
74-dic/mcl[z]		599.4* ± 0.2	1.19* ± 0.02		1	Dickinson and McLure
77-mcl/nev[aa,ee]		(599.4)		0.257 ± 0.005	7	McLure and Neville
86-fla		(599.4)	1.179		6	Flaningam
	recommended values	599 ± 1	1.19 ± 0.05	0.270 ± 0.010		
		METHYL-tris(TRIMETHYLSILOXY)SILANE (TM_3): Molar Mass 310.685 g; $C_{10}H_{30}O_3Si_4$; CASRN 17928-28-8				
57-pol	323.8 °C, 1125 cm^3·mol^{-1}	597.0*		0.276	1, 7	Pollnow

Table 2 Continued

ref	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
86-fla		(597.0)	1.182		6	Flaningam
91-chr/tra		597.4 ± 1			1	Christou et al.
	recommended values	597 ± 1	1.18 ± 0.05	0.276 ± 0.010		
	DECAMETHYLCYCLOPENTASILOXANE (D_5): Molar Mass 370.770 g; $C_{10}H_{30}O_5Si_5$; CASRN 541-02-6					
57-pol	346.0 °C, 1216 cm^3·mol^{-1}	619.2*		0.305*	1, 7	Pollnow
82-mcl/nev[dd]		617.4* ± 0.3	1.035* ± 0.02	0.288* ± 0.006	1, 7	McLure and Neville
86-fla		(619.2)	1.164*		6	Flaningam
91-chr/tra		624.8 ± 1			1	Christou et al.
	recommended values	618 ± 2	1.10 ± 0.10	0.30 ± 0.01		
	SILICIC ACID TETRAPROPYL ESTER (tetrapropoxysilane): Molar Mass 264.434 g; $C_{12}H_{28}O_4Si$; CASRN 682-01-9					
78-wat/you[x]	(16.74 ± 0.07) atm	647.7* ± 0.4	1.696*		1	Waterson and Young
2008-nik/pop		649* ± 6	1.37* ± 0.04		4	Nikitin et al.
	recommended values	648 ± 1	1.5 ± 0.2			
	HEXAETHYLDISILOXANE: Molar Mass 246.537 g; $C_{12}H_{30}OSi_2$; CASRN 994-49-0					
91-chr/tra		693.0 ± 2			1	Christou et al.
	DODECAMETHYLPENTASILOXANE (MD_3M): Molar Mass 384.839 g; $C_{12}H_{36}O_4Si_5$; CASRN 141-63-9					
57-pol	354.5 °C, 1400 cm^3·mol^{-1}	627.6*		0.275*	1, 7	Pollnow
72-you-2[y]	9.33 atm	629.0*	0.945*		1	Young
77-mcl/nev[aa]		(629.0)		0.255 ± 0.005	7	McLure and Neville
86-fla		(628.4)	0.996*			
	recommended values	628 ± 1	0.97 ± 0.05	0.275 ± 0.010		
	tetrakis(TRIMETHYLSILOXY)SILANE (QM_4): Molar Mass 384.839 g; $C_{12}H_{36}O_4Si_5$; CASRN 3555-47-3					
57-pol	350.2 °C, 1400 cm^3·mol^{-1}	623.4*		0.275	1, 7	Pollnow
86-fla		(623.35)	1.022		6	Flaningam
91-chr/tra		622.6* ± 1			1	Christou et al.
	recommended values	623 ± 1	1.0 ± 0.1	0.275 ± 0.010		
	TETRADECAMETHYLHEXASILOXANE (MD_4M): Molar Mass 458.993 g; $C_{14}H_{42}O_5Si_6$; CASRN 107-52-8					
72-you-2[y]	7.93 atm	653.2*	0.8035*		1	Young
77-mcl/nev[aa]		(653.2)		0.254 ± 0.005	7	McLure and Neville
86-fla		(653.2)	0.877*		6	Flaningam
91-chr/tra		649.9* ± 2			1	Christou et al.
	recommended values	652 ± 2	0.84 ± 0.05	0.254 ± 0.010		
	TETRADECAMETHYLCYCLOHEPTASILOXANE (D_7): Molar Mass 519.078 g; $C_{14}H_{42}O_7Si_7$; CASRN 107-50-6					
91-chr/you		683.8 ± 2			1	Christou et al.
	1,1,3,3-TETRAMETHYL-1,3-DIPHENYLDISILOXANE: Molar Mass 286.516 g; $C_{16}H_{22}OSi_2$; CASRN 56-33-7					
94-nik/pav		750 ± 8	1.73 ± 0.03		4	Nikitin et al.
	SILICIC ACID TETRABUTYL ESTER (tetrabutoxysilane): Molar Mass 320.540 g; $C_{16}H_{36}O_4Si$; CASRN 4766-57-8					
2008-nik/pop		682 ± 7	1.10 ± 0.03		4	Nikitin et al.
	HEXADECAMETHYLHEPTASILOXANE (MD_5M): Molar Mass 533.147 g; $C_{16}H_{48}O_6Si_7$; CASRN 541-01-5					
72-you-2[y]	6.68 atm	671.8*	0.677*		1	Young
86-ale	2070 cm^3·mol^{-1}	672.0*	0.760*	0.258*	3	Aleksandrova
	2023.5 cm^3·mol^{-1}	671.0*	0.648*	0.2635*		
86-fla		(671.8)	0.763*		6	Flaningam
	recommended values	671.5 ± 1.0	0.70 ± 0.10	0.260 ± 0.010		
	OCTADECAMETHYLOCTASILOXANE (MD_6M): Molar Mass 607.301 g; $C_{18}H_{54}O_7Si_8$; CASRN 556-69-4					
72-you-2[y]	6.16 atm	688.9*	0.624		1	Young
86-ale	2331 cm^3·mol^{-1}	689.7*	0.679*	0.2605	3	Aleksandrova
86-fla		(688.9)	0.677*			
	recommended values	689 ± 1	0.68 ± 0.05	0.260 ± 0.010		
	SILICIC ACID TETRAPENTYL ESTER (tetrapentoxysilane): Molar Mass 376.646 g; $C_{20}H_{44}O_4Si$; CASRN 6382-12-3					
2008-nik/pop		714 ± 7	0.89 ± 0.03		4	Nikitin et al.
	EICOSAMETHYLNONASILOXANE (MD_7M): Molar Mass 681.455 g; $C_{20}H_{60}O_8Si_9$; CASRN 2652-13-3					
86-ale		698.7*	0.563*		3	Aleksandrova
	2535.3 cm^3·mol^{-1}	698.1*	0.578*	0.2688		
	recommended values	698.5 ± 1.0	0.57 ± 0.05	0.270 ± 0.010		

Table 2 Continued

ref	values reported in nonstandard units	T_{90}/K	p/MPa	ρ/g·cm^{-3}	method	authors
	(2α,4α,6α)-2,4,6-TRIMETHYL-2,4,6-TRIPHENYLCYCLOTRISILOXANE (*cis*-...): Molar Mass 408.670 g; $C_{21}H_{24}O_3Si_3$; CASRN 3424-57-5					
94-nik/pav		824 ± 8	1.34 ± 0.03		4	Nikitin et al.
	(2α,4α,6β)-2,4,6-TRIMETHYL-2,4,6-TRIPHENYLCYCLOTRISILOXANE (*trans*-...): Molar Mass 408.670 g; $C_{21}H_{24}O_3Si_3$; CASRN 6138-53-0					
94-nik/pav		839 ± 8	1.29 ± 0.03		4	Nikitin et al.
	DOCOSAMETHYLDECASILOXANE: Molar Mass 755.609 g; $C_{22}H_{66}O_9Si_{10}$; CASRN 556-70-7					
86-ale		709.2	0.466		3	Aleksandrova
	SILICIC ACID TETRAHEXYL ESTER (tetrahexoxysilane): Molar Mass 432.753 g; $C_{24}H_{52}O_4Si$; CASRN 7425-86-7					
2008-nik/pop		757 ± 8	0.79 ± 0.02		4	Nikitin et al.
	1,3-DIMETHYL-1,1,3,3-TETRAPHENYLDISILOXANE: Molar Mass 410.655 g; $C_{26}H_{26}OSi_2$; CASRN 807-28-3					
94-nik/pav		893 ± 9	1.38 ± 0.03		4	Nikitin et al.
	SILICIC ACID TETRAHEPTYL ESTER (tetraheptoxysilane): Molar Mass 488.859 g; $C_{28}H_{60}O_4Si$; CASRN 18759-42-7					
2008-nik/pop		778 ± 8	0.74 ± 0.02		4	Nikitin et al.
	SILICIC ACID TETRAOCTYL ESTER (tetraoctoxysilane): Molar Mass 544.965 g; $C_{32}H_{68}O_4Si$; CASRN 78-14-8					
2008-nik/pop		812 ± 8	0.66 ± 0.02		4	Nikitin et al.
	SILICIC ACID TETRANONYL ESTER (tetranonoxysilane): Molar Mass 601.072 g; $C_{36}H_{76}O_4Si$; CASRN 18817-76-0					
2008-nik/pop		830 ± 8	0.61 ± 0.02		4	Nikitin et al.
	SILICIC ACID TETRADECYL ESTER (tetradecoxysilane): Molar Mass 657.178 g; $C_{40}H_{84}O_4Si$; CASRN 18845-54-0					
2008-nik/pop		849 ± 8	0.60 ± 0.02		4	Nikitin et al.

[a] Hughes et al. [59-hug/pit] measured the vapor pressure from the boiling point at 1 atm to the critical temperature, but the abstract did not provide information on how they determined the critical temperature. [b] Griskey et al. [60-gri/gor] reported slight decomposition at elevated temperatures. [c] Mousa [75-mou] repeated the results of [72-mou/kay] without citing the earlier reference. [d] Sokolova et al. [72-sok/gol] measured orthobaric densities within 3 K of T_c, but only provided an estimate for p_c, 41.2 atm (4.17 MPa), that is not reportable in Table 2. [e] Wang et al. [91-wan/adc] gave the T_c uncertainty as 0.1 K in Table 1 (p 702) but as 0.3 K on p 701, where they noted that the temperature of meniscus disappearance is established within 0.3 K. [f] Weber and Defibaugh [96-web/def] measured the vapor pressure up to 331 K and fitted their data with the Wagner equation, using the critical temperature of Schmidt et al. [96-sch/car]. [g] Values attributed to Miller [74-mil] were taken from [93-sau/hol]. Bier et al. [89-bie/tue, 90-bie/tue], who doubt that Miller's values are experimental, report a similar T_c, 226.68 °C (1968 scale), but a higher p_c, 4.93 MPa, and give 1975 as the year of publication of Miller's report. [h] Baehr et al. [89-bae/klo] accepted Bier's [87-bie] preliminary value for T_c (1968 scale), at which they determined the values of p_c and ρ_c. [i] Sauermann et al. [93-sau/hol] also used Bier's preliminary value for T_c, even though they cited [90-bie/tue] as their source. [j] Mousa [76-mou] repeated the results of [72-mou/kay], with a slight difference in ρ_c (0.5045 g·cm^{-3}), without citing the earlier reference.[j-1] Salvi-Narkhede et al. [92-sal/wan] gave the value p_c = 2.293 MPa, but the value calculated with their vapor pressure equation is 2.606 MPa. [k] Schmidt [94-sch] obtained T_c from refractive index measurements. [l] Goodwin et al. [98-goo/def] measured the vapor pressure up to 369 K and extrapolated it with the Wagner (1, 1.5, 2.5, 5) equation; when they extrapolated their measurements with the Wagner (1, 1.5, 3, 6) equation, they estimated a p_c that was higher by 62 kPa, which they took as an upper bound of the uncertainty. [m] Ambrose and Sprake [71-amb/spr] noted a rapid decomposition at the critical point. [n] The sample was stabilized after "dehydration" (drying to remove moisture). [o] The year of Throckmorton's thesis in Kudchadker et al. [68-kud/ala; ref 213] was given as 1958, and the value for the critical volume was reported as critical density. [p] Yarrington and Kay [60-yar/kay] noted that a chromatographic analysis after the completion of the measurements "showed that the sample was a mixture of close boiling isomers of indeterminate amounts... The boiling range of the sample at atmospheric pressure was approximately 0.1 °C." [q] Sinitsyn et al. [95-sin/mik] observed a gas release near the critical point. [r] Stepanov determined T_c by ultrasonic measurements [67-ste] and also p_c and ρ_c, respectively, by measuring the vapor pressure and the orthobaric densities [68-ste/noz; 72-ste]. [s] Sokolova et al. [73-sok/pro] measured orthobaric densities to within 0.5 K of T_c but only provided an estimate for p_c, 33.4 atm (3.38 MPa), that is not reportable in Table 2. [t] Anselme and Teja [90-ans/tej] could observe only one meniscus disappearance at 670 K because the sample decomposed explosively upon heating. [u] Teja and Rosenthal [91-tej/ros] also observed rapid decomposition in the flow apparatus but could determine T_c and p_c. [v] See also entry in Table 3. [w] Campbell measured the liquid density from (25 to 257) °C and estimated ρ_c without knowing T_c via Hakala's relationship: $(\rho^L + \rho^V)/2 = \rho_c + k(\rho^L - \rho^V)^{10/3}$. Campbell also gave a V_c = 237.7 cm^3·mol^{-1}, for which he may have erroneously used a molar mass of 87 g. [x] Waterson and Young [78-wat/you] also estimated the critical volumes by assuming that Z_c = 0.273. [y] Young [72-you-1, -2] also estimated the critical volume by assuming that Z_c = 0.270. [z] Dickinson and McLure [74-dic/mcl] also estimated the critical volume by assuming that $Z_c = 0.291 - 0.08\omega$ (ω: Pitzer's acentric factor [55-pit/lip]). [aa] McLure and Neville [77-mcl/nev] determined ρ_c of the first five dimethylsiloxane oligomers by fitting their liquid density data [77-mcl/pre] at approximately (298 to 413) K with the Hales-Townsend [72-hal/tow] version of the Riedel equation. For internal consistency, they used Young's [72-you-2] T_c for all of them. [bb] Osthoff and Grubb [54-ost/gru] determined ρ_c by fitting the liquid density data of Hurd [46-hur] at (273 to 353) K; in addition, they estimated a critical pressure of 14 atm (1.42 MPa) by assuming that Z_c = 0.27. [cc] Hicks and Young [71-hic/you] estimated a critical volume of 0.910 L·mol^{-1} (ρ_c = 0.326 g·cm^{-3}) by assuming that $Z_c = 0.291 - 0.08\omega$.) [dd] McLure and Neville [82-mcl/nev] determined ρ_c by fitting the liquid density data of Hurd [46-hur] at (273 to 353) K with the Hales−Townsend [72-hal/tow] version of the Riedel equation. [ee] McLure and Neville [77-mcl/nev] plotted the available experimental data for the p_c of linear dimethylsiloxane oligomers versus carbon number and concluded that the p_c of Young [72-you-2] for decamethyltetrasiloxane is too high by about 0.1 MPa. Accordingly, Young's value was not considered in the p_c recommendation.

Table 3. Critical Properties of Isocyanates Reported by Zhuravlev et al. [91-zhu/siv][a]

T_{90}/K	ρ/g·cm^{-3}
1,4-DIISOCYANATOBUTANE [$C_6H_8N_2O_2$]: Molar Mass 140.140 g; CASRN 4538-37-8	
706.7 ± 2.5	0.350 ± 0.004
1-CHLORO-6-ISOCYANATOHEXANE [$C_7H_{12}ClNO$]: Molar Mass 161.629 g; CASRN 13654-91-6	
668.9 ± 3.0	0.310 ± 0.004
1,6-DIISOCYANATOHEXANE [$C_8H_{12}N_2O_2$]: Molar Mass 168.193 g; CASRN 822-06-0	
720.8 ± 2.0	0.328 ± 0.004
1,8-DIISOCYANATOOCTANE [$C_{10}H_{16}N_2O_2$]: Molar Mass 196.246 g; CASRN 10124-86-4	
745.1 ± 4.5	0.275 ± 0.003
ISOCYANATOBENZENE (phenyl isocyanate) [C_7H_5NO]: Molar Mass 119.121 g; CASRN 103-71-9	
648.7 ± 3.0	0.401 ± 0.004
1-CHLORO-2-ISOCYANATOBENZENE [C_7H_4ClNO]: Molar Mass 153.566 g; CASRN 3320-83-0	
680.9 ± 3.0	0.460 ± 0.004
1-CHLORO-3-ISOCYANATOBENZENE [C_7H_4ClNO]: Molar Mass 153.566 g; CASRN 2909-38-8	
676.2 ± 3.0	0.479 ± 0.005
1-CHLORO-4-ISOCYANATOBENZENE [C_7H_4ClNO]: Molar Mass 153.566 g; CASRN 104-12-1	
676.9 ± 4.0	0.439 ± 0.005
1,2-DICHLORO-4-ISOCYANATOBENZENE [$C_7H_3Cl_2NO$]: Molar Mass 188.011 g; CASRN 102-36-3	
695.2 ± 4.0	0.515 ± 0.004
2,4- DIISOCYANATO-1-METHYLBENZENE [$C_9H_6N_2O_2$]: Molar Mass: 174.156 g; CASRN 584-84-9	
745.2 ± 4.0	0.415 ± 0.002

[a] Zhuravlev et al. measured the orthobaric densities and calculated from them the critical temperatures and densities, but the method of calculation is considered unsatisfactory (see text). They also provided estimates for the critical pressures. The results in Table 3 are not included in Table 1 because the T_c values do not qualify as experimental. However, see Table 2 for more recent results for the T_c and p_c of isocyanatobenzene.

Table 4. Key to Methods of Critical Point Determination

1.	Visual - in glass tube
2.	Visual - in cell with windows
3.	Nonvisual - *pVT* measurement or vapor pressure measurement
4.	Other nonvisual measurement
5.	Critical pressure measurement combined with vapor pressure measurement 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
d	decomposition at critical temperature

tigated. Until modern times, it was not possible to quantify purity, and investigators could only offer qualitative indications. Today, when methods are available for determining purity or, more correctly, the amount of impurity in a sample, a minimum mole fraction purity of 99 % is desirable, but a slightly lower purity may be acceptable if the impurities do not react with the major component and the boiling range of the sample is at most about 0.2 K. (However, see Yarrington and Kay [60-yar/kay] who discovered after completing their measurements that their sample of 2,2,3,3,4,4,5-heptafluoro-5-(nonafluorobutyl)-tetrahydrofuran, even though it had a boiling range of 0.1 K, was actually a mixture of several major components, all close-boiling isomers.)

Only critical temperatures determined according to the methods 1, 2, 3, or 4 of Table 4 are included in Table 2, although in some cases it was not possible to confirm the method used. (A minor exception was made for two compounds investigated by Sokolova et al. [1972-sok/gol, 73-sok/pro].) No estimates of T_c (or p_c) are included in Table 2, even if such estimates may agree with other experimental results. Two particular methods of estimation have been examined in earlier parts. It was demonstrated in part 6 [96-tso/amb] that T_c's estimated with the Ramsay−Shields equation from low-temperature surface tension data (method 9: *calculation* from another physical property) are generally very uncertain and should be rejected. Similarly, it was demonstrated in part 3 [1995-tso/amb] that corresponding-states estimates of T_c (and p_c) can be unreliable. As an example, consider the T_c of isocyanatobenzene (also examined in a later section): A corresponding-states prediction based on the simultaneous fit of vapor pressure and two-phase heat capacity data by Steele et al. [96-ste/chi] gave the value of 675 K, while VonNiederhausern et al. [2006-von/wil] measured the value (656.9 ± 5) K.

The critical pressures in Table 2 may have been determined with methods 1, 2, 3, or 4, but method 5 provides a confirmation of the value by combining it with vapor pressure measurements up to T_c, perhaps within *at most* 5 K of T_c, coupled with a fit of the data with a reliable vapor pressure equation; the best possible value for p_c is then the value given by the equation at T_c. But we also have the indirect method 6, where the vapor pressure measurements do not come close to T_c. In part 8 [2001-tso/amb], we argued that high-quality vapor pressure measurements even, as an example, only up to 0.27 MPa (the limit of the ebulliometric measurements at the Bartlesville, OK, laboratory) can give us reasonable p_c estimates, except for strongly associating compounds (such as alkanols and alkanoic acids). But however good the quality of measurement may be, basing p_c on a single boiling point is *not* acceptable.

Because the fluid is infinitely compressible at the critical point, direct determination of the critical density is difficult, and only a few such determinations have been made with any claim of accuracy. Critical density is normally obtained indirectly by study of the vapor−liquid coexistence curve (method 7). The orthobaric densities are obtained, and then the critical density is that given by the rectilinear diameter at the critical temperature. In the absence of another calculation method specifically for ρ_c in Table 4, method 7 may be used even when the orthobaric density measurements do not come close to T_c.

When Table 4 was drawn up, inadequate provision was made for the full range of methods to be used for critical density

determinations, which include some dependent on measurements only of liquid density: sometimes from measurements made over a wide temperature range, but at T significantly below T_c, and sometimes over a much narrower range. Consider the extensive ρ_l data of Hales and Townsend over the range about (300 to 490) K, which were combined with Riedel's generalized equation [54-rie] to obtain the ρ_c values. Their results for aromatic hydrocarbons [72-hal/tow] were discussed in part 3 and were shown to be close to values obtained by standard methods, but these values were not included in Table 2. In part 10, on the other hand, their results for fluorinated aromatic hydrocarbons [74-hal/tow] were accepted as method 7 determinations, while the ρ_c values of Sinitsyn (see next section) were not included because the values were considered to be estimates. However, as discussed in the next section, Sinitsyn et al. [96-sin/mik] also used a corresponding states approach, based on Filippov's generalized equation, and liquid density measurements up to about 90 °C, and therefore Sinitsyn's critical densities were accepted as method 7 values.

We have also accepted as method 7 critical densities the determinations of McLure and Neville [77-mcl/nev; 82-mcl/nev], who followed the approach of Hales and Townsend (see "C + H + O + Si" under "Selection of Best Values"). Method 9 critical densities included in earlier parts of this series were based on more limited liquid density measurements and no corresponding states analysis. In conclusion, method 9 should by default be reserved *only* for the estimation of ρ_c, but *no* ρ_c value has been included in Table 2 that is based on a single ρ_l measurement (at $T \ll T_c$).

Measurements by Sinitsyn

Sinitsyn et al. [95-sin/mik] reported measurements of vapor pressures, liquid densities, and some other properties for 53 fluoroorganic compounds also containing one or more of the heteroatoms O (mostly), N, and S. In addition, they reported their three critical properties, but they measured the critical temperature of only 37 of these compounds because the remaining 16 compounds either decomposed or polymerized at $T < T_c$ or for other reasons. (The uncertainty of the estimated T_c for these compounds was generally claimed to be between (10 and 20) K.) The measurements were performed in the years from 1967 to 1990, and some of the results were published in various journals. Some of the critical constants reported in [95-sin/mik] differ slightly from those in earlier publications, as they reflect final revisions made by the authors.

Sinitsyn and co-workers used the sealed ampule method for measuring the critical temperatures and the ebulliometric one for measuring the vapor pressures. As a rule, the vapor pressures were determined in the range of reduced temperatures $T_r = T/T_c$ approximately from 0.65 to 0.95. Then the critical pressures were calculated using a corresponding-states method suggested by Filippov [88-fil] that allows estimation of the critical pressure if two vapor pressures and the critical temperature are known. This approach was confirmed in this work by extrapolating the vapor pressure data with the Wagner equation.

Sinitsyn et al. also calculated the critical densities with the equation suggested by Filippov [88-fil], using their liquid density data at about (20 to 90) °C under atmospheric pressure

$$\rho_c = \rho_l \frac{1.169 + 1.792(-\log Z)}{6.444(-\log Z) - 1}, Z = \frac{P}{\rho_l RT}$$

Here R is the universal gas constant; T is the temperature; p is the vapor pressure; and ρ_l is the orthobaric molar density of the liquid or density at atmospheric pressure if the critical pressure is much higher than atmospheric. Filippov developed this equation by analyzing experimental data for a large number of well-investigated compounds, for which he calculated an uncertainty of about 0.5 % when $(-\log Z)$ varied from 1.1 to 6 and Pitzer's acentric factor ω [55-pit/lip] was in the range 0.15 to 0.75. Sinitsyn and co-workers estimate the uncertainty of the critical densities obtained by them at 1 %, but the uncertainty was raised to 2 % in the recommended values in Table 1.

Of the 19 compounds containing multiple heteroatoms (and having a purity of at least 99 %) studied by Sinitsyn et al. [95-sin/mik] that are included in Table 2, only 2,2,2-trifluoroethanol has also been investigated by others. For this particular compound, Sinitsyn's values are reasonably close to the selected T_c (within 0.7 K), p_c (0.075 MPa), and ρ_c (0.005 g·cm^{-3} or 1 %, which is Sinitsyn's estimate for all of his critical densities).

Measurements by Zhuravlev (Table 3)

The critical temperatures and densities of several isocyanates have been reported by Zhuravlev et al. [91-zhu/siv]. They measured the liquid and the vapor orthobaric densities using the sealed ampule technique (method 1 in Table 4). The authors observed thermal decomposition at elevated temperatures and ceased the measurements at temperatures from (20 to 56) K below the inferred critical temperature. The dependence of the orthobaric density on temperature was described by quadratic equations, separately for the liquid and the vapor phases, that are explicit in T

$$T = a + b\rho + c\rho^2$$

Then, by solving this system of two equations, Zhuravlev et al. obtained the critical temperature and the critical density. The form of the equation (parabola) may not be appropriate; furthermore, in some cases, the parabolas intersect (at the presumed T_c and ρ_c) but do not go through the experimental data.

Because the critical temperature was, at best, determined indirectly (and the measurements stopped, on the average, about 40 K below the inferred T_c), Zhuravlev's results are reported separately in Table 3 and are not included in Table 1. In the next section, Zhuravlev's results for isocyanatobenzene (the only one of the compounds in Table 3 that has been investigated by others) are compared with experimental data.

Selection of Best Values

Comments for individual compounds are given in Table 2 in the footnotes. Additional comments are given below.

C + H + Halogen(s) + N. Mustafaev et al. [96-mus/ima] determined the T_c and p_c of four perfluorinated N compounds (and one perfluorinated O compound); see Literature Cited and Table 2. The purity of the samples was stated to be over 99 %, while the uncertainty was determined to be not more than 1 % for the vapor pressure and 1.5 % for the critical properties. The maximum uncertainty is reasonable for p_c (about 0.02 MPa) but is surprisingly large, (7 to 9) K, for a method 1 T_c (direct observation of the meniscus disappearance or appearance in a sealed ampule).

Additional data are available for only one of the compounds investigated by Mustafaev et al., perfluorotributylamine (the much longer IUPAC name is given in the registry and the tables), and the difference in T_c is substantial (less so in p_c). Toczylkin and Young [80-toc/you] reported 565.42 K (corrected to the ITS-90 scale) and 1.16 MPa, that is, about 4.3 K and 0.06 MPa higher than the corresponding results of Mustafaev et al. The recommended values in Tables 1 and 2 are close to

those of Toczylkin and Young, whose measurements on other compounds generally have uncertainties of <0.5 K and <0.05 MPa.

C + H + Halogen(s) + O. 2,2,2-Trifluoroethanol. This compound gained considerable interest in the 1980s, especially in Germany and Japan, as a working fluid in refrigeration cycles and heat pumps. Several papers dealing with such applications report estimates for the critical properties of 2,2,2-trifluoroethanol. Table 2 lists only experimental data, although it was not possible to ascertain the source of Miller's [74-mil] values. The investigation of Bier et al. [89-bie/tue, 90-bie/tue] appears to be the most carefully done, and thus their T_c (the only one for which the temperature scale correction was used) and p_c values are recommended.

Fluoroethers. The concern over global warming led to the development, primarily in Japan, of a new generation of refrigerants that may be even better than the hydrofluorocarbons that are currently replacing the conventional hydrochlorofluorocarbon refrigerants. Among these new-generation refrigerants are the fluoroethers. Table 2 reports new data for 33 fluoroethers. The search for new refrigerants extended to fluoroketones and even fluoroamines.

As shown in Table 2, several Japanese groups have investigated a few of the fluoroethers, which can establish the quality of measurements for many more fluoroethers and other compounds where only a single investigation was made. In addition, several Japanese papers report values for critical constants that have been reported previously. An example of this is the paper of Yasumoto et al. [2007-yas/uch], which reports critical constants that have already been published.

C + H + Halogens + Si. Smith [94-smi] tabulates T_c's and p_c's for aromatic compounds containing Cl and Si that are claimed to be unpublished Dow Corning Corp. data, but Flaningam [99-fla] has confirmed that all these values were calculated with Lydersen's method.

C+ H + N + O. Two investigations, one in 1946 and the other in 2002, have used variations of an old technique. Griffin [49-gri] employed the method of Cailletet and Colardeau to determine the critical properties of *nitromethane*. As discussed in part 1 [95-amb/you], Cailletet and Colardeau in 1888, and again Ipatieff and Monroe in 1942, measured the pressure in a bomb, that is, a constant-volume apparatus. If the bomb was filled correctly, as the temperature was raised, the vapor pressure curve would show a corner (a break in the slope of the vapor pressure) at the critical temperature, but this is a relatively insensitive method. A variation of this method used by Glaser and Rüland in 1957 was briefly reviewed in part 3 [95-tso/amb].

Wilson et al. [2002-wil/von] measured the T_c and p_c of *2-[(2-aminoethyl)amino]ethanol* with a *new* "ultra-low residence time" flow method that was described by VonNiederhausern et al. [2000-von/wil]. This new method bears some similarities with the earlier methods but has the advantage, because of being able to reduce the residence time down to 0.1 s, of being applicable to thermally unstable substances. It is based on making temperature scans in the vicinity of the critical point. When these are plotted as T(fluid) versus T(bath), a horizontal region indicative of isothermal boiling will be observed below the critical point. "The critical point is inferred by the temperature and pressure where isothermal boiling is no longer observed." Although "assigning the critical point can be somewhat subjective," the error has been minimized by taking several temperature scans at small intervals. Additional measurements on several compounds with this method are reported by VonNiederhausern et al. [2004-von/gil, 2006-von/wil].

The second of these papers [2006-von/wil] reports the T_c and p_c of *isocyanatobenzene* (phenyl isocyanate): (656.9 ± 5) K and (4.00 ± 0.20) MPa. The T_c of this compound is also included in Table 3: (648.7 ± 3.0) K. Although Zhuravlev's [91-zhu/siv] value is about 8 K below the accepted value, the difference is equal to the sum of the two uncertainties. On the other hand, as mentioned earlier, a corresponding-states prediction based on the simultaneous fit of vapor pressure and two-phase heat capacity data by Steele et al. [96-ste/chi] gave the much higher value of 675 K. (The last two references also report p_c and ρ_c estimates.)

Kudchadker et al. [68-kud/ale] report the T_c of isoxazole from Speroni et al. [47-spe/pin], but this value, 552 K, is not included in Table 2 because it was calculated from room-temperature surface tension measurements (see third paragraph under "What Should Be Included in Table 2?").

C + H + O + Si. The names of the poly(dimethylsiloxane) oligomers are very long, but a very useful shorthand system of nomenclature introduced by Wilcock [46-wil] can maintain clarity and conciseness. The simple compounds are made up of **M**, the monofunctional terminal group $(CH_3)_3SiO_{1/2}$, and **D**, the bifunctional repetitive unit $(CH_3)_2SiO$. Thus, all simple linear molecules are written as $MD_{x-2}M$ (or M_2D_{x-2}) and all cyclic molecules are written as D_x, where x is the total number of silicon-containing units. Branchiness can be introduced by **T**, the trifunctional group $CH_3SiO_{3/2}$, and **Q**, the tetrafunctional group SiO_2. For poly(diphenysiloxane) oligomers, **D*** represents the bifunctional group $(C_6H_5)_2SiO$.

Poly(dimethylsiloxane) oligomers. Flaningam [86-fla], as part of his experimental determination of the vapor pressure of linear and cyclic dimethylsiloxane oligomers, collected available data (and estimates) for their critical properties. Especially useful are the unpublished T_c and ρ_c data of Pollnow [57-pol], which were measured at Dow Corning. Although the methods were not given in [86-fla], Morgan [2005-mor] confirmed that they were measured, respectively, by method 1 and method 7. Flaningam also tabulated, but rejected, Pollnow's estimates for the critical pressure and Cholpan's [64-cho] estimates for the critical temperature. These estimates are not reported here.

In addition to reporting the unpublished data of Pollnow, Flaningam measured the vapor pressure of 16 poly(dimethyl)-siloxanes and extrapolated them to what he considered to be the best T_c (in 1986). The resulting p_c's (with method 6) for compounds that have experimentally determined T_c's are included in Table 2 and are generally close to available experimental data.

McLure and Neville [77-mcl/nev] determined the critical density of five linear dimethylsiloxane oligomers by fitting liquid density data at approximately (298 to 413) K by McLure et al. [77-mcl/pre] with the Hales−Townsend [72-hal/tow] version of the Riedel equation. The uncertainty for the resulting critical densities, which are included in Table 2 (method 7), was estimated at 2 %. Although they used the same approach for hexadecamethylheptasiloxane and octadecamethyloctasiloxane, they only had for each compound a single liquid density value at 298.15 K [1946-hun/war]. The resulting critical densities, respectively, (0.250 and 0.246) $g \cdot cm^{-3}$, are not included in Table 2 because it is our position that a single liquid density value at room temperature should not suffice to determine ρ_c—just as a single boiling point should not be all that is required to determine p_c.

McLure and Neville [82-mcl/nev] also used the same approach to calculate the critical density of octamethylcyclotetrasiloxane and decamethylcyclopentasiloxane, for which they

used the liquid density data of Hurd [46-hur] at (273 to 353) K. The uncertainty was estimated at 2 %.

Very recently, Nikitin et al. [2008-nik/pop] used their pulse-heating method to determine the T_c and p_c of the first ten tetraalkyl esters of silicic acid, all thermally unstable at the critical point. Their results for the first three esters agree, within the stated uncertainties, with the values of Waterson and Young [78-wat/you], except for their p_c result for the tetrapropyl ester, which is significantly lower.

Finally, Nikitin et al. [88-nik/pav] have measured the T_c and p_c of industrial polyethylsiloxanes. These liquids are not considered in this series of reviews because they are mixtures of a variety of molecules of varying degree of polymerization and structure.

A Final Check

As a final check, we examined the compounds in Table 1 that have values for $Z_c > 0.3$ or < 0.2. The former would be unlikely for nonpolar compounds, while $Z_c < 0.2$ is possible for large nonpolar molecules. However, much less is known about the Z_c of polyfunctional compounds such as those examined in part 11. In any case, the most likely sources of erratic Z_c's are poor p_c or ρ_c values, as the percentage error in T_c is generally small.

As an example of how uncertainty in ρ_c affects the value of Z_c, consider the Z_c values calculated from the results of Mousa et al. [72-mou/kay, 75-, 76-, 81-mou]: trifluoroethanenitrile ($Z_c = 0.283$), hexafluoro-2-propanone (0.311), and 1,1,1,5,5,5-hexafluoro-2,4-pentanedione (0.198). Part 10 [2007-mar/abr] included measurements by Mousa for three fluorinated hydrocarbons, for which Mousa's critical densities were off the selected values by 0.05 $g \cdot cm^{-3}$, which was assumed as the uncertainty in his part 11 results. Such a large uncertainty is supported by the investigation of Główka and Zawisza [69-glo/zaw], who reported for hexafluoro-2-propanone a $\rho_c = 0.576$ $g \cdot cm^{-3}$, a value that is significantly higher than Mousa's 0.505 $g \cdot cm^{-3}$. Using the average value 0.54 $g \cdot cm^{-3}$ lowered Z_c to 0.294, the value listed in Table 1.

Two fluorinated acids have nearly identical Z_c's: trifluoroethanoic acid (0.163), investigated by Zawisza [67-zaw], and the more complex 2,4,6,8-tetraoxaheptadecafluorononanoic acid (0.164), investigated by Sinitsyn et al. [95-sin/mik]; also see above under Measurements by Sinitsyn. Sinitsyn et al. also investigated 2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoroheptanol ($Z_c = 0.309$).

Also, high Z_c's are reported for pentafluoro(trifluoromethyl)sulfur (0.302), investigated by Beyerlein et al. [98-bey/des], and pentafluoro(1,1,2,2-tetrafluoroethoxy)ethane (0.311), investigated by Sako et al. [98-sak/yas]. CF_8S is the only C−F−S compound for which p_c and ρ_c have been measured, and thus little can be said about such compounds. However, Sako et al. and several other Japanese investigators have produced high-quality critical property data for fluoroethers, and thus it would be difficult to question the quality of their results.

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Registry Numbers Supplied by the Authors

Boric acid trimethyl ester, 121-43-7; trifluoroethanenitrile, 353-85-5; difluoro-*N,N*-bis(trifluoromethyl)methanamine, 73563-15-2; *N,N*-bis(trifluoromethyl)methanamine,85034-09-9; 2,2-difluoro-*N,N*-bis(trifluoromethyl)ethanamine, 176674-31-0; *N,N*-bis(trifluoromethyl)ethanamine, 85034-08-8; 1,1,2,2,3,3,3-heptafluoro-*N,N*-bis(heptafluoropropyl)-1-propanamine, 338-83-0; 1,1,2,2,3,3,4,4,4-nonafluoro-*N*-nonafluorobutyl-*N*-(trifluoromethyl)-1-butanamine, 514-03-4; 2,2,3,3,4,4,4a,5,5,6,6,7,7,8,8,8a-hexadecafluorodecahydro-1-(pentafluoroethyl)quinoline, 130539-68-3; 1,1,-2,2,3,3,4,4,4-nonafluoro-*N,N*-bis(nonafluorobutyl)-1-butanamine, 311-89-7; trichloroacetyl chloride, 76-02-8; trifluoroethanoic acid, 76-05-1; difluoromethoxytrifluoromethane, 3822-68-2; oxy-bis(difluoromethane), 1691-17-4; 2,2,2-trifluoroethanol, 75-89-8; trifluoromethoxymethane, 421-14-7; chloropentafluoro-2-propanone, 79-53-8; hexafluorooxetane, 425-82-1; hexafluoro-2-propanone, 684-16-2; trifluoro(trifluoromethyl)oxirane, 428-59-1; hexafluoro-1,3-dioxolane, 21297-65-4; pentafluoro(trifluoromethoxy)ethane, 665-16-7; difluoro-bis(trifluoromethoxy) methane, 53772-78-4; 1,1,1,2-tetrafluoro-2-(trifluoromethoxy)ethane, 2356-62-9; 1,1,2,2-tetrafluoro-1-(trifluoromethoxy)ethane, 2356-61-8; 2-chloro-1-(difluoromethoxy)-1,1,2-trifluoroethane, 13838-16-9; 2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane, 26675-46-7; 1,1,1-trifluoro-2-(trifluoromethoxy)ethane, 20193-67-3; 1,1,1,2-tetrafluoro-2-(difluoromethoxy)ethane, 57041-67-5; 1,1,1-trifluoro-2-(difluoromethoxy)ethane, 1885-48-9; 1,2,2-trifluoro-2-(difluoromethoxy)ethane, 69948-24-9; pentafluoro(methoxy)ethane, 22410-44-2; 2,2,3,3-tetrafluoro-1-propanol, 76-37-9; carbonchloridic acid ethyl ester, 541-41-3; 1,1,1-trifluoro-2-(methoxy)ethane, 460-43-5; octafluorotetrahydrofuran, 773-14-8; 1,1,1,2,2,3,3-heptafluoro-3-(trifluoromethoxy)propane, 59426-77-6; 2,2,3,3,5,5,6-heptafluoro-1,4-dioxane, 34118-18-8; 4,4,5,5-tetrafluoro-2-(trifluoromethyl)-1,3-dioxolane, 269716-57-6; pentafluoro(1,1,2,2-tetrafluoroethoxy)ethane, 134769-21-4; pentafluoro(2,2,2-trifluoroethoxy)ethane, 156053-88-2; 1,1,1,3,3,3-hexafluoro-2-(difluoromethoxy)propane, 26103-08-2; 1,1-bis-(difluoromethoxy)-1,2,2,2-tetrafluoroethane, 267901-02-0; 3,3,4,4,4-pentafluoro-2-butanone, 374-41-4; 3-difluoromethoxy-1,1,1,2,2-pentafluoropropane, 56860-81-2; 1,1,1,2,2,3,3-heptafluoro-3-(methoxy)propane, 375-03-1; 1,1,1,2,3,3,3-heptafluoro-2-(methoxy)propane, 22052-84-2; 1,1,2,2-tetrafluoro-1-(2,2,2-trifluoroethoxy)ethane, 406-78-0; 1,1,1,3,3,3-hexafluoro-2-(methoxy)propane, 13171-18-1; 1,1,2,2-tetrafluoro-2-(2,2-difluoroethoxy)ethane, 50807-77-7; 1,1,1-trifluoro-2-(2,2,2-trifluoroethoxy)ethane, 333-36-8; pentafluoro(ethoxy)ethane, 22052-81-9; 3-methoxy-1,1,2,2-tetrafluoropropane, 60598-17-6; nonafluoropentanoyl fluoride, 375-62-2; nonafluoropentanoic acid, 2706-90-3; 1,1,1,5,5,5-hexafluoro-2,4-pentanedione, 1522-22-1; 1,1,1,2,4,4,4-heptafluoro-2-(trifluoromethoxy)butane, 347148-74-7; 1,1,1,2,2,3,3-heptafluoropentan-4-one, 355-17-9; 3,4,4,4-tetrafluoro-3-(trifluoromethyl)-2-butanone, 80553-01-1; 1,1,1,2,3,3-hexafluoro-3-(2,2,2-trifluoroethoxy)propane, 993-95-3; 1,1,1,3,3,3-hexafluoro-2-trifluoromethyl-2-(methoxy)propane, 66670-22-2; 2,2,3,3,4,4,5,5,5-nonafluoro-1-pentanol,355-28-2; 1,1,1,2,2-pentafluoro-3-(1,1,2,2-tetrafluoroethoxy)propane, 50807-74-4; 2,2,3,3,4,4,5,5-octafluoro-1-pentanol, 355-80-6; 1,1,2,2-tetrafluoro-3-(1,1,2,2-tetrafluoroethoxy)propane, 16627-68-2; 1,1,1,2,2-pentafluoropentan-3-one, 378-72-3; 4-methoxy-1,1,1,2,2,3,3-heptafluorobutane, 376-98-7; pentafluorophenol, 771-61-9; 1,1,1,2,2,3,3,4,4-nonafluorohexan-5-one, 678-18-2; 1,1,1,2,3,3-hexafluoro-3-(2,2,3,3,3-pentafluoropropoxy)propane, 1000-28-8; 2,2,3,3,4,4,5,5-octafluoropentanoic acid methyl ester, 54822-22-9; 1,1,1,2,3,3-

hexafluoro-3-(2,2,3,3-tetrafluoropropoxy)propane, 65064-78-0; 4-ethoxy-1,1,1,2,2,3,3,4,4-nonafluorobutane, 16370-05-4; tridecafluoroheptanoyl chloride, 52447-22-0; 2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoro-1-heptanol, 375-82-6; 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-1-heptanol, 355-99-9; 1,1,2,2,3,3,4,4-octafluoro-5-(1,1,2,2-tetrafluoroethoxy)pentane, 16627-71-7; 3,3,4,4,5,5,6,6-octafluoro-2-methyl-2-hexanol, 2673-15-6; 1,1,5-trichloro-2,2,3,3,4,4,5,5-octafluoro-1-(1,1,1,2,3,3-hexafluoro-2-chloropropoxy)pentane, 912670-61-2; 2,2,3,3,4,4,5-heptafluoro-5-(nonafluorobutyl)tetrahydrofuran, 335-36-4;1-[1-[difluoro-(pentafluoroethoxy)methyl]-1,2,2,2-tetrafluoroethoxy]-1,1,2,2,3,3,3-heptafluoropropane, 66804-94-2; 1,1,2,2-tetrafluoroethoxybenzene, 350-57-2; 2,4,6,8-tetraoxaheptadecafluorononanoic acid, 252556-93-7; 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoroheptanoic acid ethyl ester, 42287-85-4; octafluoro-1,4-butanedisulfonyl difluoride, 84246-31-1; pentafluoro(trifluoromethyl)sulfur, 373-80-8; thio-bis-trifluoromethane, 371-78-8; trichloromethylsilane, 75-79-6; trichloroethylsilane, 115-21-9; dichlorodimethylsilane, 75-78-5; chlorotrimethylsilane, 75-77-4; dichlorodiethylsilane, 1719-53-5; nitromethane, 75-52-5; 2-aminoethanol, 141-43-5; 1,3-oxazole, 288-42-6; *N,N*-dimethylformamide, 68-12-2; *N*-methylacetamide, 79-16-3; 2-(2-aminoethoxy)ethanol, 929-06-6; 2,2′-imino-bis-ethanol, 111-42-2; 2-[(2-aminoethyl)amino]ethanol, 111-41-1; 1-methyl-2-pyrrolidinone, 872-50-4; 4-formylmorpholine, 4394-85-8; 3-methyl-1-nitrosooxybutane, 110-46-3; *N*-methyldiethanolamine, 105-59-9; 2,2′,2″-nitrilo-tris-ethanol, 102-71-6; isocyanatobenzene, 103-71-9; 1-cyclohexyl-2-pyrrolidinone, 6837-24-7; sulfinyl-bis-methane, 67-68-5; ethanethioic acid S-ethyl ester, 625-60-5; silicic acid tetramethyl ester, 681-84-5; hexamethyldisiloxane, 107-46-0; hexamethylcyclotrisiloxane, 541-05-9; 1,1,1,3,5,5,5-heptamethyltrisiloxane, 1873-88-7; silicic acid tetraethyl ester, 78-10-4; octamethyltrisiloxane, 107-51-7; octamethylcyclotetrasiloxane, 556-67-2; decamethyltetrasiloxane, 141-62-8; methyl-tris(trimethylsiloxy)silane, 17928-28-8; decamethylcyclopentasiloxane, 541-02-6; silicic acid tetrapropyl ester, 682-01-9; hexaethyldisiloxane, 994-49-0; dodecamethylpentasiloxane, 141-63-9; tetrakis(trimethylsiloxy)silane, 3555-47-3; tetradecamethylhexasiloxane, 107-52-8; tetradecamethylcycloheptasiloxane, 107-50-6; 1,1,3,3-tetramethyl-1,3-diphenyldisiloxane, 56-33-7; silicic acid tetrabutyl ester, 4766-57-8; hexadecamethylheptasiloxane, 541-01-5; octadecamethyloctasiloxane, 556-69-4; silicic acid tetrapentyl ester, 6382-12-3; eicosamethylnonasiloxane, 2652-13-3; (2α,4α,6α)-2,4,6-trimethyl-2,4,6-triphenylcyclotrisiloxane,3424-57-5;(2α,4α,6β)-2,4,6-trimethyl-2,4,6-triphenylcyclotrisiloxane, 6138-53-0; docosamethyldecasiloxane, 556-70-7; silicic acid tetrahexyl ester, 7425-86-7; 1,3-dimethyl-1,1,3,3-tetraphenyldisiloxane, 807-28-3; silicic acid tetraheptyl ester, 18759-42-7; silicic acid tetraoctyl ester, 78-14-8; silicic acid tetranonyl ester, 18817-76-0; silicic acid tetradecyl ester, 18845-54-0.

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2001-yos/miz Yoshii, Y.; Mizukawa, M.; Widiatmo, J. V.; Watanabe, K. *J. Chem. Eng. Data* **2001**, *46*, 1050−1053 (pentafluoro(methoxy)ethane).

2002-wil/von Wilson, G. M.; VonNiederhausern, D. M.; Giles, N. F. *J. Chem. Eng. Data* **2002**, *47*, 761−764 (2-[(2-aminoethyl)amino]ethanol).

2003-kay Kayukawa, Y. Private communication, 2003 (trifluoromethoxymethane).

2003-kay/has Kayukawa, Y.; Hasumoto, M.; Hondo, T.; Kano, Y.; Watanabe, K. *J. Chem. Eng. Data* **2003**, *48*, 1141−1151 (trifluoromethoxymethane, pentafluoro(methoxy)ethane).

2003-ota/yas Otake, K.; Yasumoto, M.; Yamada, Y.; Murata, J.; Urata, S. *J. Chem. Eng. Data* **2003**, 48, 1380−1383 (2,2-difluoro-*N,N*-bis(trifluoromethyl)ethanamine; 1,1,1,2,2,3,3-heptafluoropentan-4-one, 1,1,1,2,2-pentafluoropentan-3-one, 1,1,1,2,2,3,3,4,4-nonafluorohexan-5-one); also presented approximate results for a partially stable hydrofluoroketone.

2003-yas/yam Yasumoto, M.; Yamada, Y.; Murata, J.; Urata, S.; Otake, K. *J. Chem. Eng. Data* **2003**, *48*, 1368−1379 (3-difluoromethoxy-1,1,1,2,2-pentafluoropropane, 1,1,2,2-tetrafluoro-1-(2,2,2-trifluoroethoxy)ethane, 1,1,2,2-tetrafluoro-2-(2,2-difluoroethoxy)ethane, 1,1,1-trifluoro-2-(2,2,2-trifluoroethoxy)ethane, 3-methoxy-1,1,2,2-tetrafluoropropane, 1,1,1,2,3,3-hexafluoro-3-(2,2,2-trifluoroethoxy)propane, 1,1,1,2,2-pentafluoro-3-(1,1,2,2-tetrafluoroethoxy)propane, 1,1,2,2-tetrafluoro-3-(1,1,2,2-tetrafluoroethoxy)propane, 4-methoxy-1,1,1,2,2,3,3-heptafluorobutane, 1,1,1,2,3,3-hexafluoro-3-(2,2,3,3,3-pentafluoropropoxy)propane, 4-ethoxy-1,1,1,2,2,3,3,4,4-nonafluorobutane); also presented approximate results for 4 partially stable hydrofluoroethers (their Table 7).

2004-ota/uch Otake, K.; Uchida, Y.; Yasumoto, M.; Yamada, Y.; Furuya, T.; Ochi, K. *J. Chem. Eng. Data* **2004**, *49*, 1643−1647 (pentafluoro(methoxy)ethane).

2004-uch/yas Uchida, Y.; Yasumoto, M.; Yamada, Y.; Ochi, K.; Furuya, T.; Otake, K. *J. Chem. Eng. Data* **2004**, *49*, 1615−1621 (trifluoromethoxymethane).

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