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Selected Physicochemical Properties of Hexamethylcyclotrisiloxane, Octamethylcyclotetrasiloxane, and Decamethylcyclopentasiloxane

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Liquid densities, viscosities, orthobaric heat capacities, surface tensions, thermal conductivities, and saturated vapor pressures were measured for samples of mole fraction purity of 99.98 % HMCTS, OMCTS, and DMCPS over wide temperature ranges, by using Anton Paar densimeter, Hoeppler viscosimeter, Perkin-Elmer DSC 1B, modified bubble method, "hot wire" technique, and comparative ebulliometry, respectively. The experimental data were correlated and deviations or, for vapor pressure data, overall measures of data reproducibility are given.

Introduction

Cyclic dimethylsiloxanes are still receiving attention both due to their wide range of practical applications and theoretical interest. Poly(dimethylsiloxanes) are used in different industrial, technical, and medical applications. Forming approximately spherical or ellipsoidal molecules siloxanes, they are interesting from a theoretical point of view. An exception is hexamethylcyclotrisiloxane that possesses a planar, strained ring structure and, when compared to other cyclic dimethylsiloxanes, has a relatively high melting point and short liquid range. Among cyclic siloxanes properties of pure octamethylcyclotetrasiloxane have been thoroughly investigated. For other siloxanes, information is usually limited to some fundamental properties, like saturated vapor pressures and/or densities. In this paper, results of measurements of several properties over wide temperature ranges are presented for the first three cyclic dimethylsiloxanes.

Experimental Section

Chemicals. A laboratory substance, 99 %, was dried for 48 h over 4 Å molecular sieves and then rectified through a 35-theoretical plate column. A forerun, about 25 %, was collected at a reflux ratio of 1:30. The major fraction was collected within the boiling temperature range of ± 0.005 K. The resulting product had a mole fraction purity 99.98 %. It was found by Fischer's method to contain 0.02 % mass fraction of water. Gas chromatography showed no other contaminants to be present. This product was used for the physicochemical measurements.

Density. An Anton Paar densimeter DMA 60/DMA 602H was used to measure the density over a temperature range of (343.15 to 387.85) K for HMCTS, (292.00 to 433.15) K for OMCTS, and (295.05 to 453.15) K for DMCPS, respectively. The temperature of the measuring cell in the densimeter was controlled by a thermostat with a circulating medium to within ± 0.03 K. A precision quartz thermometer was used to read the cell temperature to an uncertainty of ± 0.015 K. The oscillation period (τ) in the vibrating U-tube of the densimeter was converted to density by using the following equation

$$\rho = A(\tau^2 - B) \tag{1}$$

where A and B constants were established by using the literature data for pure water and dry air. The uncertainty in the density measurement was estimated to be ± 0.01 $\text{kg}\cdot\text{m}^{-3}$. Data are listed in Table 1. The experimental values were correlated by the linear equations:

$$\text{for HMCTS:}\quad \rho/\text{kg}\cdot\text{m}^{-3} = 1321.29 - 1.30728T/\text{K} \tag{2a}$$

$$\text{for OMCTS:}\quad \rho/\text{kg}\cdot\text{m}^{-3} = 1303.79 - 1.18562T/\text{K} \tag{2b}$$

$$\text{for DMCPS:}\quad \rho/\text{kg}\cdot\text{m}^{-3} = 1281.57 - 1.10088T/\text{K} \tag{2c}$$

with standard deviations as follows: $\sigma(\rho/\text{kg}\cdot\text{m}^{-3}) = 0.36$ for HMCTS, $\sigma(\rho/\text{kg}\cdot\text{m}^{-3}) = 0.14$ for OMCTS, $\sigma(\rho/\text{kg}\cdot\text{m}^{-3}) = 0.07$ for DMCPS. Graphs of residuals between corresponding experimental and calculated values plotted versus temperature indicate for all the three substances some parabolic tendency in distribution, but statistical analysis does not support the importance of the quadratic term.

Viscosity. Viscosity was measured with a Hoeppler viscosimeter over a temperature range of (343.15 to 393.15) K for HMCTS, (293.15 to 423.15) K for OMCTS, and (293.15 to 493.15) K for DMCPS, respectively. The measurements uncertainty was estimated to be ± 0.005 mPa·s. The temperature of viscosimeter was controlled to within ± 0.05 K. Data are listed in Table 2. The experimental data were correlated with the equations:

$$\text{for HMCTS:}\quad \ln(\eta/\text{mPa}\cdot\text{s}) = -4.0074 + \frac{1124.2}{T/\text{K}} \tag{3a}$$

$$\text{for OMCTS:}\quad \ln(\eta/\text{mPa}\cdot\text{s}) = -4.8920 + \frac{1698.7}{T/\text{K}} \tag{3b}$$

$$\text{for DMCPS:}\quad \ln(\eta/\text{mPa}\cdot\text{s}) = -4.8747 + \frac{1855.5}{T/\text{K}} \tag{3c}$$

Standard deviations are equal $\sigma(\eta/\text{mPa}\cdot\text{s}) = 0.003$ for HMCTS, $\sigma(\eta/\text{mPa}\cdot\text{s}) = 0.009$ for OMCTS, and $\sigma(\eta/\text{mPa}\cdot\text{s})$

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Table 1. Experimental Results for Liquid Density, ρ and $\Delta\rho$ ($=\rho_{\mathrm{exp}} - \rho_{\mathrm{calc}}$), of Hexamethylcyclotrisiloxane (HMCTS), Octamethylcyclotetrasiloxane (OMCTS), and Decamethylcyclopentasiloxane (DMCPS)

HMCTS			OMCTS			DMCPS		
T	ρ	$\Delta\rho$	T	ρ	$\Delta\rho$	T	ρ	$\Delta\rho$
K	$\mathrm{kg \cdot m^{-3}}$	$\mathrm{kg \cdot m^{-3}}$	K	$\mathrm{kg \cdot m^{-3}}$	$\mathrm{kg \cdot m^{-3}}$	K	$\mathrm{kg \cdot m^{-3}}$	$\mathrm{kg \cdot m^{-3}}$
343.15	872.69	−0.01	292.00	957.55	−0.04	295.05	956.75	−0.01
348.70	865.41	−0.03	301.60	946.16	−0.05	300.10	951.14	−0.06
354.65	856.98	−0.68	303.15	944.21	−0.16	303.95	946.93	−0.03
357.40	854.11	0.04	311.20	934.80	−0.03	310.30	939.94	−0.03
359.15	852.60	0.82	313.15	932.43	−0.08	313.17	936.67	−0.14
366.10	842.76	0.07	316.00	929.12	−0.01	320.50	928.72	−0.02
369.65	838.00	−0.05	325.62	917.74	0.01	325.60	923.12	−0.00
373.15	833.47	−0.01	330.47	912.06	0.08	333.15	915.02	0.21
379.16	825.64	0.02	333.15	909.32	0.52	340.90	906.30	0.02
383.15	820.39	−0.02	340.05	900.68	0.06	346.05	900.69	0.08
387.85	814.16	−0.10	344.80	894.99	−0.00	353.10	892.80	−0.05
			349.65	889.31	0.07	366.40	878.24	0.03
			353.15	884.79	−0.30	373.15	870.77	−0.01
			364.04	872.24	0.06	381.70	861.40	0.03
			373.15	861.35	−0.03	391.90	850.17	0.03
			383.20	849.47	0.01	397.00	844.55	0.03
			393.15	837.64	−0.02	407.20	833.32	0.03
			397.60	832.37	−0.02	413.15	826.73	−0.01
			407.22	821.00	0.02	417.40	822.08	0.02
			413.15	813.94	−0.01	422.50	816.45	0.00
			421.58	803.91	−0.05	433.15	804.71	−0.02
			433.15	790.24	−0.00	442.90	793.98	−0.01
						453.15	782.60	−0.11

Table 2. Experimental Results for Liquid Viscosity, η and $\Delta\eta$ ($=\eta_{\mathrm{exp}} - \eta_{\mathrm{calc}}$), of Hexamethylcyclotrisiloxane (HMCTS), Octamethylcyclotetrasiloxane (OMCTS), and Decamethylcyclopentasiloxane (DMCPS)

HMCTS			OMCTS			DMCPS		
T	η	$\Delta\eta$	T	η	$\Delta\eta$	T	η	$\Delta\eta$
K	$\mathrm{mPa \cdot s}$	$\mathrm{mPa \cdot s}$	K	$\mathrm{mPa \cdot s}$	$\mathrm{mPa \cdot s}$	K	$\mathrm{mPa \cdot s}$	$\mathrm{mPa \cdot s}$
343.15	0.48	−0.001	293.15	2.45	−0.016	293.15	4.28	−0.004
348.15	0.46	0.001	303.15	2.06	0.023	298.15	3.87	0.018
353.15	0.44	0.001	313.15	1.70	−0.003	303.15	3.48	0.003
358.15	0.42	0.000	323.15	1.44	0.000	313.15	2.82	−0.039
363.15	0.40	−0.002	333.15	1.23	0.000	323.15	2.38	−0.000
368.15	0.39	0.005	343.15	1.06	0.000	332.95	2.02	0.010
373.15	0.37	0.000	353.15	0.92	−0.001	343.15	1.71	0.007
378.15	0.35	−0.006	363.15	0.81	0.003	353.15	1.48	0.019
383.15	0.34	−0.002	373.15	0.71	−0.002	373.15	1.11	0.007
388.15	0.33	0.001	383.15	0.63	−0.002	393.15	0.86	0.004
393.15	0.32	0.003	393.15	0.56	−0.005	413.15	0.69	0.009
			403.15	0.51	0.003	423.15	0.57	−0.043
			423.15	0.41	−0.006	453.15	0.46	0.002
						473.15	0.39	0.004
						493.15	0.33	0.001

= 0.018 for DMCPS, respectively. Like in the case of density data, graphs of residuals for viscosity plotted versus temperature show some parabolic tendency in distribution. This behavior suggests use of the Antoine's equation for description of data; however, statistical analysis in all the cases does not support this expectation.

Liquid Heat Capacity. Heat capacity was measured over a temperature range of (339.90 to 404.89) K for HMCTS, (293.15 to 425.95) K for OMCTS, and (288.78 to 473.15) K for DMCTS by a DSC-1B Perkin-Elmer differential scanning microcalorimeter. The temperature was controlled to within ± 0.05 K. The uncertainty in the liquid heat capacity measurement was estimated to be ± 0.01 $\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$. Sapphire of purity 99.9999 % was used as a standard. The experimental data (Table 3) were correlated by the use of the equations:

$$\text{for HMCTS:}\quad C_p/\mathrm{J \cdot mol^{-1} \cdot K^{-1}} = 254.5 + 0.4413T/\mathrm{K} \tag{4a}$$

$$\text{for OMCTS:}\quad C_p/\mathrm{J \cdot mol^{-1} \cdot K^{-1}} = 385.15 + 0.43105T/\mathrm{K} \tag{4b}$$

$$\text{for DMCPS:}\quad C_p/\mathrm{J \cdot mol^{-1} \cdot K^{-1}} = 499.68 + 0.48083T/\mathrm{K} - 2.565 \cdot 10^{-5}(T/\mathrm{K})^2 \tag{4c}$$

Standard deviations are equal $\sigma(C_p/\mathrm{J \cdot mol^{-1} \cdot K^{-1}}) = 0.13$ for HMCTS, $\sigma(C_p/\mathrm{J \cdot mol^{-1} \cdot K^{-1}}) = 0.16$ for OMCTS, and $\sigma(C_p/\mathrm{J \cdot mol^{-1} \cdot K^{-1}}) = 0.06$ for DMCPS, respectively. Parameters of eq 4b were obtained excluding two points, and parameters of eq 4c were obtained excluding four points (marked with asterisk in Table 3). These points are statistical outliers at the 95 % confidence level. Standard deviation for OMCTS with all points accounted for equals $\sigma(C_p/\mathrm{J \cdot mol^{-1} \cdot K^{-1}}) = 0.56$ and for DMCPS equals $\sigma(C_p/\mathrm{J \cdot mol^{-1} \cdot K^{-1}}) = 0.42$.

Thermal Conductivity. Thermal conductivity was measured at 343.15 K for HMCTS and at (298.15 and 343.15) K for OMCTS and DMCPS by a comparative-type transient "hot wire" apparatus similar to that described by Mallan et al.[27] The measuring cell was a water-jacketed capillary, which made a double-step precision thermostating possible. A thin platinum wire (15 cm long and 0.01 cm in diameter) was placed concentrically inside the capillary, which was placed in a Wheatstone bridge circuit to determine λ from measurements upon the heat source alone. The capillary was filled with investigated liquid, and electric current was passed at varying intensities. At each intensity the resistance of the wire was measured. The calibration constants for the measuring cell were evaluated from measurements carried out for water and benzene as standard liquids. The uncertainty in the thermal conductivity measurement was estimated to be ± 0.1 $\mathrm{mW \cdot m^{-1} \cdot K.^{-1}}$

The data for OMCTS and DMCPS measured at 293.15 K and for HMCTS, OMCTS, and DMCPS at 343.15 K are listed in Table 5.

Surface Tension. Surface tension was measured over a temperature range of (344.55 to 383.15) K for HMCTS, (293.15 to 433.15) K for OMCTS, and (293.15 to 433.15) K for DMCTS by the maximum bubble pressure method. The operating principle of this method has been presented by Kihm and Degnan.[28] The method involves the measurements of the pressure differential developed within the system as bubbles of dry air presaturated with vapor are drawn alternately through two glass capillaries of diameters (4.0 and 0.5) mm, respectively, immersed to the same depth in a liquid. The pressure differential is developed by a mercury aspirator and measured on a water-filled manometer. The uncertainty in the surface tension measurements was tested by measuring the surface tension for distilled and deionized water and was estimated to be ±,0.01 $\mathrm{mN \cdot m^{-1}}$. The experimental data (Table 4) were correlated by the use of the equations:

$$\text{for HMCTS:}\quad \gamma/\mathrm{mN \cdot m^{-1}} = 35.239 - 0.06304T/\mathrm{K} \tag{5a}$$

$$\text{for OMCTS:}\quad \gamma/\mathrm{mN \cdot m^{-1}} = 38.50 - 0.0700T/\mathrm{K} \tag{5b}$$

$$\text{for DMCPS:}\quad \gamma/\mathrm{mN \cdot m^{-1}} = 37.935 - 0.06779T/\mathrm{K} \tag{5c}$$

Standard deviations are equal: $\sigma(\gamma/\mathrm{mN \cdot m^{-1}}) = 0.02$ for HMCTS, $\sigma(\gamma/\mathrm{mN \cdot m^{-1}}) = 0.03$ for OMCTS, and $\sigma(\gamma/\mathrm{mN \cdot m^{-1}}) = 0.03$ for DMCPS, respectively.

Table 3. Experimental Results for Liquid Heat Capacity, C_p and ΔC_p ($=C_{p,\mathrm{exp}} - C_{p,\mathrm{calc}}$), of Hexamethylcyclotrisiloxane (HMCTS), Octamethylcyclotetrasiloxane (OMCTS), and Decamethylcyclopentasiloxane (DMCPS)[a]

HMCTS			OMCTS			DMCPS		
T	C_p	ΔC_p	T	C_p	ΔC_p	T	C_p	ΔC_p
K	$\mathrm{J{\cdot}mol^{-1}{\cdot}K^{-1}}$	$\mathrm{J{\cdot}mol^{-1}{\cdot}K^{-1}}$	K	$\mathrm{J{\cdot}mol^{-1}{\cdot}K^{-1}}$	$\mathrm{J{\cdot}mol^{-1}{\cdot}K^{-1}}$	K	$\mathrm{J{\cdot}mol^{-1}{\cdot}K^{-1}}$	$\mathrm{J{\cdot}mol^{-1}{\cdot}K^{-1}}$
339.90	404.5	0.0	293.15	511.5	−0.0	288.78	636.3	−0.1
343.15	405.9	−0.1	298.00	513.6	−0.0	293.13	638.5	0.1
345.03	406.7	−0.1	303.15	515.8	−0.0	297.95	640.6	−0.1
353.15	410.4	0.0	306.25	517.2	0.0	303.18	643.1	0.0
357.92	412.3	−0.2	313.12	520.1	−0.0	308.95	644.5	−1.3*
361.20	413.8	−0.1	319.00	522.7	0.0	313.15	647.7	−0.0
365.09	415.6	0.0	323.25	524.5	0.0	319.00	650.4	−0.1
370.16	418.1	0.2	327.55	526.4	0.1	323.15	652.4	0.0
374.79	420.1	0.2	334.75	529.1	−0.3	329.05	655.1	−0.0
379.42	421.8	−0.2	337.88	530.8	0.0	334.74	657.9	0.1
383.15	423.6	0.0	342.23	532.7	0.0	338.50	659.5	−0.0
388.06	425.6	−0.2	348.05	535.2	0.0	342.08	661.2	0.0
393.14	428.1	0.1	352.20	538.8	1.8*	349.25	664.5	0.0
398.01	430.0	−0.2	358.83	539.9	0.1	352.20	667.1	1.3*
400.00	431.0	0.0	364.28	542.2	0.0	356.83	668.0	0.0
404.89	433.2	0.0	370.25	543.0	−1.7*	361.28	670.1	0.1
			377.55	548.0	0.1	366.35	672.4	0.0
			382.48	550.1	0.1	370.25	674.2	0.0
			388.65	552.3	−0.4	375.43	676.6	0.0
			393.15	554.7	0.1	380.95	679.1	−0.0
			399.83	557.7	0.2	388.65	682.5	−0.2
			407.15	560.8	0.2	391.43	684.0	0.0
			415.73	564.5	0.2	399.84	687.9	0.1
			425.95	568.4	−0.4	401.55	688.6	−0.0
						407.15	691.2	−0.0
						412.77	693.8	0.0
						419.95	697.1	0.0
						425.95	698.5	−1.3*
						433.28	703.2	−0.0
						439.98	706.3	0.0
						444.90	709.2	0.7*
						452.40	711.9	−0.1
						463.15	716.9	0.0
						469.05	719.5	−0.1
						473.15	721.5	0.1

[a] Asterisk (*) indicates excluded data points in eqs 4b and 4c.

Table 4. Experimental Results for Surface Tension, γ and $\Delta\gamma$ ($=\gamma_{\mathrm{exp}} - \gamma_{\mathrm{calc}}$), of Hexamethylcyclotrisiloxane (HMCTS), Octamethylcyclotetrasiloxane (OMCTS), and Decamethylcyclopentasiloxane (DMCPS)

HMCTS			OMCTS			DMCPS		
T	γ	$\Delta\gamma$	T	γ	$\Delta\gamma$	T	γ	$\Delta\gamma$
K	$\mathrm{mN{\cdot}m^{-1}}$	$\mathrm{mN{\cdot}m^{-1}}$	K	$\mathrm{mN{\cdot}m^{-1}}$	$\mathrm{mN{\cdot}m^{-1}}$	K	$\mathrm{mN{\cdot}m^{-1}}$	$\mathrm{mN{\cdot}m^{-1}}$
344.55	13.54	0.02	293.15	17.93	−0.05	293.15	18.04	−0.02
347.35	13.32	−0.02	303.15	17.28	−0.00	303.15	17.40	0.02
353.95	12.90	−0.02	313.15	16.60	0.02	313.15	16.71	0.00
358.45	12.68	0.04	323.15	15.95	0.07	323.15	15.99	−0.04
363.15	12.33	−0.01	333.15	15.16	−0.02	333.15	15.42	0.07
368.15	12.02	−0.01	343.15	14.50	0.02	343.15	14.67	−0.00
373.15	11.71	−0.00	353.15	13.77	−0.01	353.15	13.98	−0.01
378.15	11.40	0.00	363.15	13.05	−0.03	363.15	13.30	−0.02
383.15	11.09	0.01	373.15	12.38	0.00	373.15	12.64	0.00
			393.15	10.98	−0.00	393.15	11.28	−0.00
			413.15	9.58	−0.00	413.15	9.93	0.00
			433.15	8.18	−0.00	433.15	8.57	−0.00

Vapor Pressure. Saturated vapor pressure was measured over a temperature range of (347.64 to 407.63) K for HMCTS, (311.80 to 446.26) K for OMCTS, and (348.23 to 479.53) K for DMCTS, respectively. The comparative ebulliometric technique comprising a dynamic twin-ebulliometer assembly was used as described elsewhere.[1] Temperature was measured on ITS-90 with a platinum resistance thermometer (Leeds & Northrup, model 8163-C) operated in conjunction with a Mueller bridge (Leeds & Northrup, type G-2) and an electronic null detector (Leeds & Northrup, model 9834). To provide replicate data, each equilibrium point was measured six times. The maximum uncertainty in the temperature measurement and the associated pressure inconstancy were estimated at ± 5 mK and ± 6.7 Pa, respectively. To obtain the fits to the Antoine equation:

$$\text{for HMCTS:}\quad \ln(P/\mathrm{kPa}) = 13.47185 - \frac{2906.90}{T/\mathrm{K} - 79.496} \tag{6a}$$

$$\text{for OMCTS:}\quad \ln(P/\mathrm{kPa}) = 12.92945 - \frac{2751.94}{T/\mathrm{K} - 115.354} \tag{6b}$$

$$\text{for DMCPS:}\quad \ln(P/\mathrm{kPa}) = 12.67409 - \frac{2772.84}{T/\mathrm{K} - 135.502} \tag{6c}$$

The maximum likelihood method was used as described

Table 5. Experimental Results for Liquid Thermal Conductivity, λ, of Hexamethylcyclotrisiloxane (HMCTS), Octamethylcyclotetrasiloxane (OMCTS), and Decamethylcyclopentasiloxane (DMCPS)

HMCTS		OMCTS		DMCPS	
T	λ	T	λ	T	λ
K	$mW\cdot m^{-1}\cdot K^{-1}$	K	$mW\cdot m^{-1}\cdot K^{-1}$	K	$mW\cdot m^{-1}\cdot K^{-1}$
		298.15	113.1	298.15	125.5
343.15	102.6	343.15	103.8	343.15	118.6

Table 6. Experimental Temperatures, T, Orthobaric Pressures, P, Precision Measures, σ_T and σ_P, Calculated Residuals, ΔT ($=T_{exp} - T_{calc}$) and ΔP ($=P_{exp} - P_{calc}$), and Overall Measures of Data-Point Reproduction, κ, of Hexamethylcyclotrisiloxane (HMCTS) from (347.64 to 407.63) K

T/K	σ_T/K	ΔT/K	P/kPa	σ_P/kPa	ΔP/kPa	κ
347.64	0.009	−0.061	13.849	0.002	0.005	−1.47
350.13	0.010	−0.078	15.277	0.004	0.021	−1.89
351.45	0.005	0.028	16.191	0.002	−0.007	1.32
355.59	0.010	0.038	19.006	0.002	−0.002	0.79
360.17	0.015	0.019	22.549	0.001	0.000	0.25
361.61	0.005	−0.003	23.754	0.001	0.000	−0.12
362.40	0.009	0.021	24.470	0.002	−0.001	0.49
365.71	0.010	0.085	27.619	0.001	−0.001	1.72
368.81	0.012	0.009	30.711	0.004	−0.001	0.16
372.34	0.005	−0.012	34.633	0.004	0.007	−0.58
372.68	0.009	−0.032	35.009	0.005	0.008	−0.78
381.37	0.009	−0.004	46.626	0.006	0.001	−0.11
383.78	0.012	−0.010	50.313	0.003	0.000	−0.17
387.95	0.009	−0.027	57.217	0.004	0.003	−0.63
397.75	0.030	−0.009	76.516	0.053	0.013	−0.08
407.63	0.010	0.024	100.848	0.003	−0.001	0.49

Table 7. Experimental Temperatures, T, Orthobaric Pressures, P, Precision Measures, σ_T and σ_P, Calculated Residuals, ΔT ($=T_{exp} - T_{calc}$) and ΔP ($=P_{exp} - P_{calc}$), and Overall Measures of Data-Point Reproduction, κ, of Octamethylcyclotetrasiloxane (OMCTS) from (311.80 to 446.23) K

T/K	σ_T/K	ΔT/K	P/kPa	σ_P/kPa	ΔP/kPa	κ
311.80	0.010	0.034	0.355	0.001	−0.014	2.12
317.63	0.009	0.008	0.535	0.003	−0.026	1.25
318.25	0.008	0.004	0.548	0.003	−0.017	0.84
328.59	0.010	−0.014	0.988	0.004	0.036	−1.33
328.78	0.012	−0.022	0.996	0.004	0.039	−1.46
332.94	0.012	−0.035	1.295	0.003	0.028	−1.45
336.67	0.011	0.001	1.642	0.003	−0.001	0.05
339.58	0.009	−0.004	1.926	0.002	0.002	−0.14
343.99	0.008	−0.008	2.426	0.004	0.016	−0.60
349.86	0.005	−0.022	3.277	0.002	0.021	−1.68
360.26	0.008	0.044	5.470	0.003	−0.025	1.47
376.51	0.009	0.039	10.955	0.002	−0.004	0.72
379.31	0.009	0.003	12.228	0.001	0.000	0.06
381.23	0.008	−0.019	13.172	0.001	0.001	−0.36
383.17	0.010	0.046	14.237	0.002	−0.003	0.72
383.58	0.011	0.017	14.443	0.001	0.000	0.23
388.92	0.012	0.049	17.674	0.004	−0.008	0.67
389.73	0.013	0.037	18.202	0.006	−0.012	0.51
390.88	0.009	−0.045	18.904	0.003	0.007	−0.82
396.28	0.010	−0.006	22.946	0.004	0.001	−0.09
407.56	0.010	−0.034	33.457	0.005	0.008	−0.54
413.82	0.011	−0.011	40.803	0.004	0.001	−0.15
423.24	0.014	−0.008	54.111	0.005	0.001	−0.08
446.26	0.009	0.005	100.820	0.005	−0.001	0.09

Table 8. Experimental Temperatures, T, Orthobaric Pressures, P, Precision Measures, σ_T and σ_P, Calculated Residuals, ΔT ($=T_{exp} - T_{calc}$) and ΔP ($=P_{exp} - P_{calc}$), and Overall Measures of Data-Point Reproduction, κ, of Decamethylcyclopentasiloxane (DMCPS) from (348.23 to 479.53) K

T/K	σ_T/K	ΔT/K	P/kPa	σ_P/kPa	ΔP/kPa	κ
348.23	0.010	0.016	0.703	0.001	−0.004	0.77
350.87	0.009	−0.008	0.801	0.003	0.018	−1.13
351.11	0.008	−0.004	0.820	0.003	0.011	−0.69
355.91	0.005	0.000	1.103	0.004	−0.003	0.16
357.29	0.008	0.005	1.207	0.004	−0.018	0.83
361.20	0.009	−0.006	1.468	0.003	0.008	−0.50
370.08	0.010	0.036	2.381	0.003	−0.027	1.81
374.37	0.011	0.022	2.913	0.002	−0.005	0.60
377.85	0.012	0.024	3.452	0.004	−0.017	0.86
378.07	0.009	0.032	3.482	0.002	−0.010	1.11
380.74	0.010	−0.038	3.901	0.003	0.019	−1.35
394.66	0.009	−0.030	7.191	0.002	0.005	−0.78
398.63	0.005	−0.037	8.450	0.001	0.004	−1.59
402.72	0.006	−0.022	9.938	0.001	0.002	−0.76
412.81	0.007	0.012	14.519	0.002	−0.002	0.38
416.46	0.008	0.053	16.555	0.001	−0.001	1.25
423.94	0.010	0.047	21.386	0.004	−0.011	1.01
432.91	0.012	0.071	28.603	0.006	−0.020	1.25
439.98	0.013	0.046	35.465	0.003	−0.002	0.67
448.41	0.014	0.012	45.279	0.004	−0.001	0.17
455.39	0.010	−0.042	54.850	0.005	0.007	−0.83
462.39	0.010	−0.017	66.094	0.004	0.002	−0.32
479.53	0.012	−0.008	100.896	0.005	0.001	−0.13

in more detail elsewhere.[1,2] Tables 6 (for HMCTS), 7 (for OMCTS), and 8 (for DMCPS) list the observed (T_i, P_i) data pairs, their estimated precision measures ($\sigma_{T,s}$, $\sigma_{P,s}$), and the deviations (ΔT_i, ΔP_i) between the observed and calculated variables. The ΔT_i, ΔP_i values allow us to check whether the values obtained for error variances are appropriate, by assessing whether the variations in these fall properly within their (computed) confidence intervals. Since neither ΔT_i nor ΔP_i alone is adequately representative as an overall measure of reproduction for an individual data point, we suggested the following:[1]

$$\kappa_i^{s} = \mathrm{sgn}(\Delta T_i)\cdot\kappa_i/\hat{\sigma} \tag{7}$$

where, for the present case,

$$\kappa_i = [(\Delta P_i/\sigma_{P_i})^2 + (\Delta T_i/\sigma_{T_i})^2]^{1/2} \tag{8}$$

as an overall measure of data point reproduction, where κ_i is the distance between the ith observed and estimated data points in the (P, T) space, σ_T and σ_P are adopted as length units. The κ_i^s values are seen (eq 7) to be scaled with respect to $\hat{\sigma}$ (i.e., to the standard deviation of κ_i) given by

$$\hat{\sigma} = \left[\sum_{i=1}^{n}\kappa_i^{2}/(n-3)\right]^{1/2} \tag{9}$$

where n is the number of experimental points. The sign of ΔT_i has been attributed to κ_i to have the experimental point located ”below” or ”above” the response curve. When systematical errors are absent, sign of κ_i^s should be randomly distributed, and absolute values should be about unity; large κ_i values ($\gg 1$) may indicate outliers. Easy measure of the randomness of κ_i^s is the number of sign changes test. If two neighboring κ_i^s have opposite signs, then one speaks of a sign change. Total number of sign changes should be roughly equal to $n/2 \pm (n/2)^{1/2}$ (limits at 68 % probability level). The corresponding values are 5 (5 to 11) for HMCTS, 15 (8 to 16) for OMCTS, and 15 (8 to 14) for DMCPS, where values in parentheses are limits calculated at 68 % probability level.

The calculated deviations (Tables 6, 7, and 8) in observed temperature (ΔT) and pressure (ΔP) show a consistently statistical pattern, and especially as regards temperature, they do not rise in the vicinity to the normal boiling point. This shows that the substance is thermally stable and shows no signs of decomposition as the temperature is

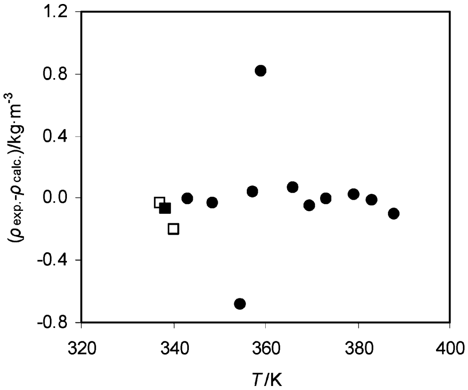

Figure 1. HMCTS. Deviations between the experimental densities and the values calculated with eq 2a vs temperature: ●, this work; ■, Fischer and Weiss;[3] □, Fischer and Weiss[3] (calculated from reported parameters).

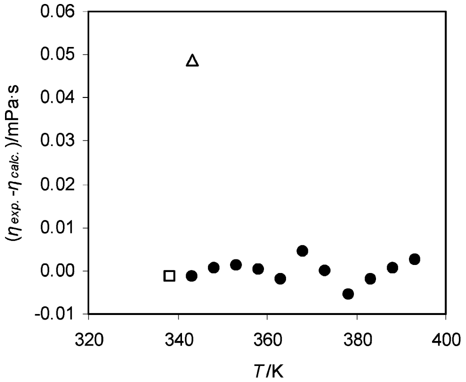

Figure 2. HMCTS. Deviations between the experimental viscosities and the values calculated with eq 3a vs temperature: ●, this work; □, Fischer and Weiss;[3] △, Waterman et al.[15]

increased. Indirectly, this fact is also a confirmation of the high purity of the sample used for the measurements.

Results and Discussion

To our knowledge, values for the liquid thermal conductivity for all the three siloxanes, the surface tension for HMCTS are for the first time measured and reported in this work. Other properties measured can be compared with corresponding literature data. Deviations between the experimental data, both the newly measured and taken from literature, and the values calculated with relevant equations with parameters fitted to the new data versus temperature are presented in Figures 1 to 15.

Density for HMCTS can be compared with corresponding values calculated from parameters reported by Fischer and Weiss[3] fitted to data measured in the range (337 to 340) K and a single experimental data measured by Fischer and Weiss at 338.2 K. The calculated values and the experimental one agreed excellently with the new data.

For OMCTS density was measured by Hurd[9] (specific volumes) in the range (273 to 353) K, Marsh[4] at 293.15 K (for five data points in the range (298 to 333) K parameters of second-order polynomial are reported), Myers and Clever[10] in the range (293 to 318) K, Levien and Marsh[5] at (298.15 and 318.15) K, Young[7] at (503 to 576.3) K, Marsh (1971)[19] at 586.5 K, Herring and Winnick[8] in the range (298 to 424) K, Fischer and Weiss[3] at 298 K (reported parameters fitted to four temperatures in the range (290 to 340) K), McLure and Barbarín-Castillo[6] (orthobaric specific volumes) at (292 to 408) K. Wappmann et al.[11] reported densities measured between 294 K and 433 K at pressures up to 180 MPa. At the lowest temperatures, all the measured values agreed to within 0.5 kg·m.$^{-3}$ For higher temperatures, the present data can be compared with the corresponding data of McLure and Barbarín-Castillo.[6] Deviations for the data of McLure and Barbarín-Castillo[6] form approximately parabolic shape with a maximum deviation of 2 kg·m^{-3} at the middle of temperature range and excellent agreement at both ends.

For DMCPS, density was measured by Hurd[9] (reported specific volumes) in the range (273 to 353) K, Hunter et al.[13] at 298.15 K, Waterman et al.[15] at 293.15 K, and

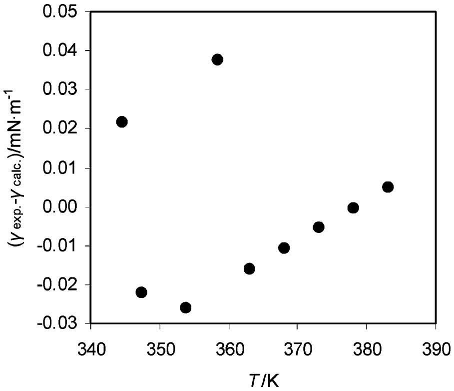

Figure 3. HMCTS. Deviations between the experimental surface tensions and the values calculated with eq 4a vs temperature: ●, this work.

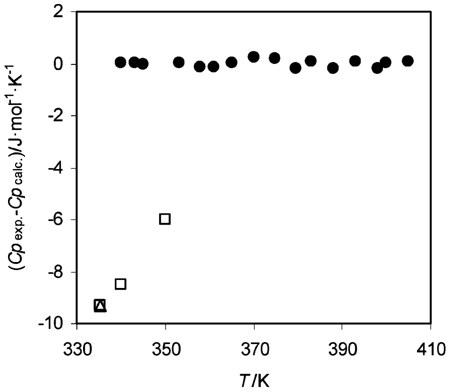

Figure 4. HMCTS. Deviations between the experimental orthobaric molar heat capacities and the values calculated with eq 5a vs temperature: ●, this work; □, Kuliev et al.;[24] △, Kuliev et al.[29]

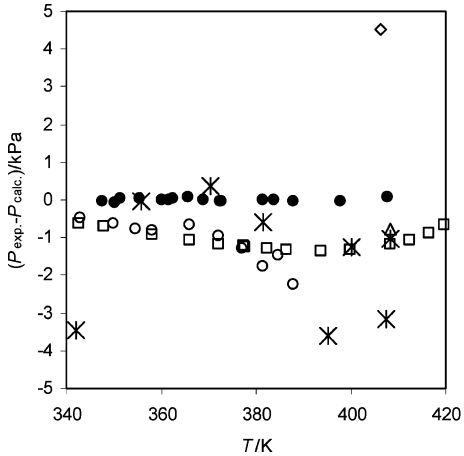

Figure 5. HMCTS. Deviations between the experimental saturated vapor pressures and the values calculated with eq 6a vs temperature: ●, this work; ◇, Hunter et al.;[13] ○, Osthoff et al.;[17] △, Waterman et al.;[15] *, Ditsent et al.;[25] □, Flaningam.[18]

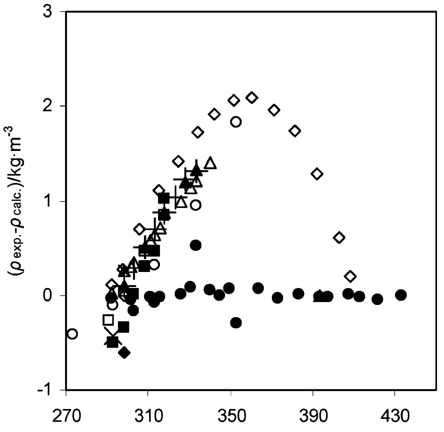

Figure 6. OMCTS. Deviations between the experimental densities and the values calculated with eq 2b vs temperature: ●, this work; ○, Hurd;[3] ◆, Hunter et al.;[13] ■, Myers and Clever;[10] ×, Wappmann et al.;[11] ▲, Marsh;[4] □, Livien and Marsh;[5] +, Herring and Winnick;[8] △, Fischer and Weiss;[3] ◇, McLure and Barbarín-Castillo.[6]

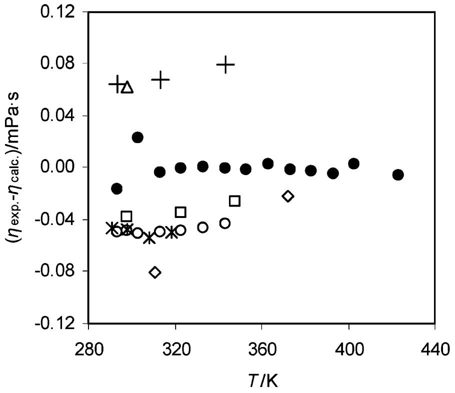

Figure 7. OMCTS. Deviations between the experimental viscosities and the values calculated with eq 3b vs temperature: ●, this work; □, Hurd;[9] △, Hunter et al.;[13] ◇, Wilcock;[12] +, Waterman et al.;[15] *, Marsh;[23] ○, Fischer and Weiss.[3]

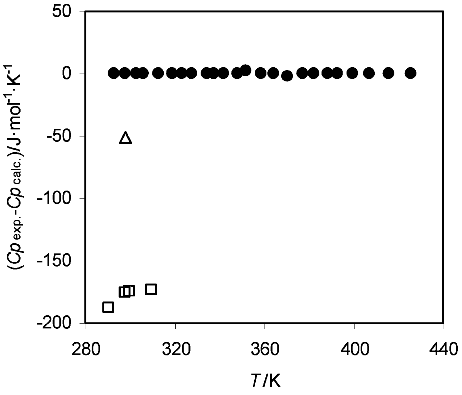

Figure 8. OMCTS. Deviations between the experimental orthobaric molar heat capacities and the values calculated with eq 4b vs temperature: ●, this work; △, Marsh and Tomlins;[14] □, Mekhtiev et al.[26]

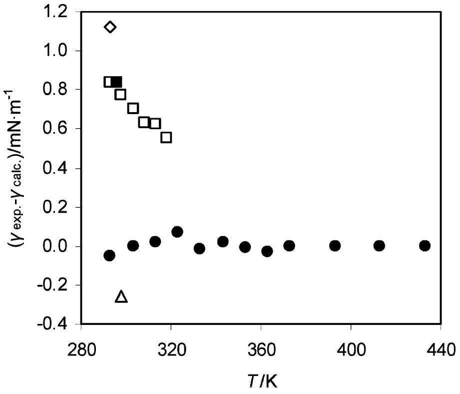

Figure 9. OMCTS. Deviations between the experimental surface tensions and the values calculated with eq 5b vs temperature: ●, this work;; △, Hunter et al.;[13] ◇, Waterman et al.;[15] □, Myers and Clever;[10] ■, Lam et al.[16]

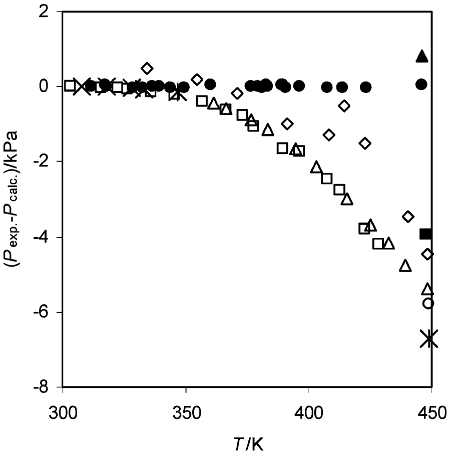

Figure 10. OMCTS. Deviations between the experimental saturated vapor pressures and the values calculated with eq 6b vs temperature: ●, this work; ■, Hurd;[9] *, Wilcock;[12] □, Osthoff et al.;[17] ▲, Waterman et al.;[15] ×, Marsh;[4] +, Hurd;[9] ◇, Ditsent et al.;[25] △, Flaningam.[18]

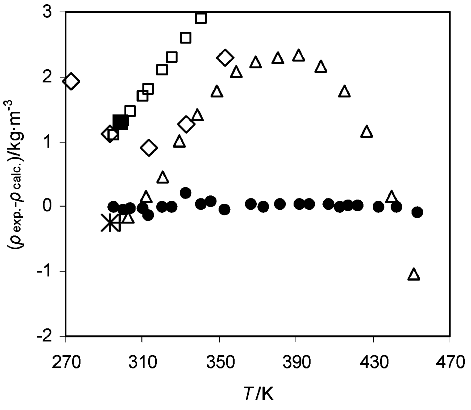

Figure 11. DMCPS. Deviations between the experimental densities and the values calculated with eq 2c vs temperature: ●, this work; ◇, Hurd;[9] +, Hunter et al.;[13] *, Waterman et al.;[15] ■, Fischer and Weiss;[3] □; Fischer and Weiss[3] (calculated from reported parameters); Δ, McLure and Barbarín-Castillo.[6]

Fischer and Weiss[3] at 298.2 K. Fischer and Weiss reported parameters fitted to four temperatures in the range (290 to 340) K. McLure and Barbarín-Castillo[6] reported orthobaric specific volumes measured in the range (302 to 451) K. The values calculated using parameters reported by Fischer and Weiss exhibit systematic linear shift of deviations reaching the value of 2.9 kg·m^{-3} at 340 K. Deviations for data of McLure and Barbarín-Castillo[6] form approximately parabolic shape with maximum deviation of 2.3 kg·m^{-3} at the middle of temperature range and excellent agreement at both ends.

Viscosity for HMCTS can be compared with experimental data measured at Fischer and Weiss[3] at 338.2 K, and Waterman et al.[15] measured at 343.15 K. Fischer and Weiss[3] reported parameters of the linear equation. If there

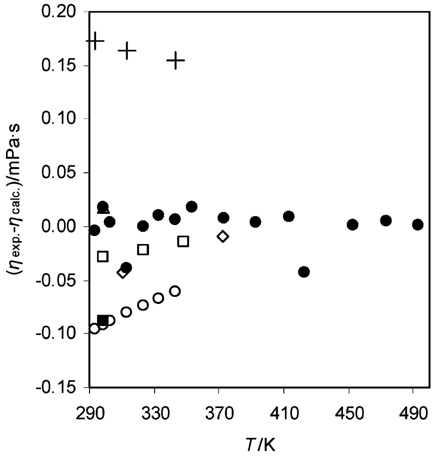

Figure 12. DMCPS. Deviations between the experimental viscosities and the values calculated with eq 3c vs temperature: ●, this work; □, Hurd;[9] △, Hunter et al.;[13] ◇, Wilcock;[12] +, Waterman et al.;[15] ■, Fischer and Weiss;[3] ○, Fischer and Weiss[3] (calculated from reported parameters).

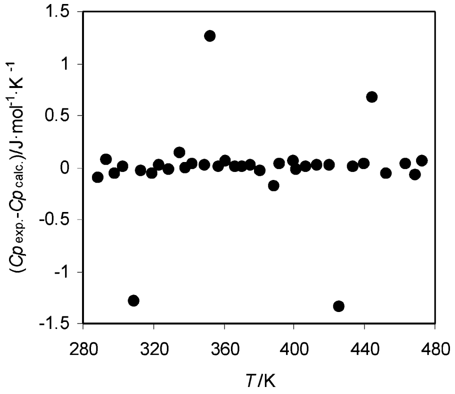

Figure 13. DMCPS. Deviations between the experimental orthobaric molar heat capacities and the values calculated with eq 4c vs temperature: ●, this work.

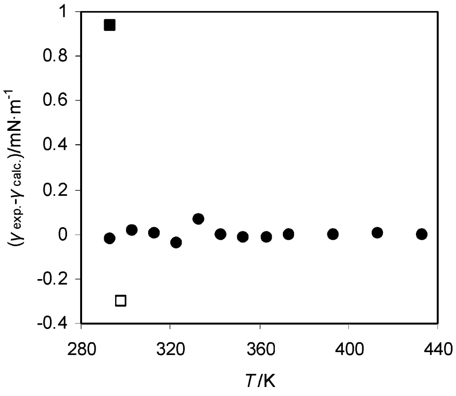

Figure 14. DMCPS. Deviations between the experimental surface tensions and the values calculated with eq 5c vs temperature: ●, this work; □, Hunter et al.;[13] ■, Waterman et al.[15]

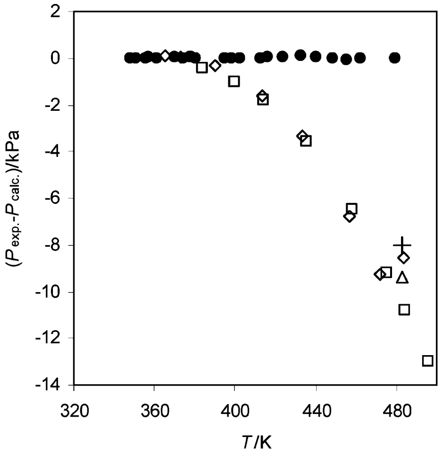

Figure 15. DMCPS. Deviations between the experimental saturated vapor pressures and the values calculated with eq 6c vs temperature: ●, this work; +, Hurd;[9] ◇, Ditsent et al.;[25] □, Flaningam;[18] △, Fischer and Weiss.[3]

is no misprint, the reported parameters were fitted to data measured in the range (338.2 to 340) K. So, the reliability out of this range should be rather poor. The reported value at 338.2 K excellently agrees with the value calculated using eq 3a. For OMCTS viscosity was measured by Hurd[9] at (298, 323, and 348) K, Wilcock[12] at (311 and 372) K, Hunter et al.[13] at 298.15 K, Marsh[23] in the range (291 to 318) K, Waterman et al.[15] at (293.15, 313.15, and 343.15) K, Fischer and Weiss[3] at 298.2 K (reported parameters fitted data measured in the range (285 to 340) K). The present values are (on average 0.05 mPa·s) higher than those reported in the literature except for the value reported by Hunter et al.[13] and Waterman et al.[15] for which the maximum deviation is 0.086 mPa·s.

For DMCPS viscosity was measured by Hurd[9] at (298, 323, and 348) K, Wilcock[12] at (311 and 372) K, Hunter et al.[13] at 298.15 K, Fischer and Weiss[3] at 298.2 K, and Waterman et al.[15] at (293.15, 313.15, and 343.15) K. Fischer and Weiss[3] reported also parameters fitted to data measured in the range (285 to 340) K. The new results agree with literature data within experimental error except for the value reported by Fischer and Weiss[3] (difference −0.087 mPa·s) and Waterman et al.[15] (the maximum difference 0.173 mPa·s). The values calculated from reported parameters are smaller than the recent data and asymptotically tends with the rise of temperature to our data.

The new heat capacity data for HMCTS agreed well with the data of Dow Corning listed in the DIPPR 801 database.[30] Kuliev et al.[24] reported experimental data at (335.22, 340, and 350) K and Kuliev et al.[29] at 335 K. These data are systematically lower than new measurements of about 8 J·mol^{-1}·K.$^{-1}$

Single approximate value for the heat capacity of OMCTS has been reported by Marsh and Tomlins[14] equal to 1.56 J·cm^{-3}·K^{-1} at 298.15 K. Their molar liquid heat capacity equals to 463 J·mol^{-1}·K^{-1} and is about 51 J·mol^{-1}·K^{-1} lower than obtained in our experiment. Mekhtiev et al.[26] reported experimental data in the range (290.55 to 310) K. These data are systematically lower than the new measurements of about 175 J·mol^{-1}·K.$^{-1}$ Since the recent data are comparable with those of Dow Corning, thus there must be some error in data reported by Mekhtiev et al.[26] There are literature data for DMCPS, but we have not succeeded to extract these values from the literature. From referee's comments: results that the new data for DMCPS agreed with those of Dow Corning.

Surface tension of OMCTS was measured by Hunter et al.[13] at 298.15 K, Waterman et al.[15] at 293.15 K, Myers and Clever[10] in the range (293 to 318) K, and Lam et al.[16] at 296.2 K. Except for the point measured by Hunter et al.,[13] all the literature data are systematically higher about (0.6 to 0.9) mN·m^{-1}, which much more than exceeded estimated experimental error. The value of Hunter et al.[13] is slightly below our value. The new data, according to the referee's comments, are comparable with those of Dow Corning.

For DMCPS, we have found only two experimental values reported in the literature measured by Hunter et al.[13] at 298.15 K and Waterman et al.[15] at 293.15 K. First is slightly below the new value, and the latter is 1 $mN\cdot m^{-1}$ above. The new data, according to the referee's comment, "fit in well with the trend at lower temperature" with proprietary data of Dow Corning.

Saturated vapor pressures were investigated for all compounds. For HMCTS, Hunter et al.[13] reported value of the normal boiling point, Osthoff et al.[17] reported saturated vapor pressures in the range (303 to 428) K, Waterman et al.[15] reported the normal boiling temperature, Flaningam[18] reported saturated vapor pressures in the range (342 to 420) K, and Ditsent et al.[25] reported saturated vapor pressures in the range (342 to 408) K. Generally, the new data are systematically higher of about 1 kPa.

For OMCTS Hurd[9] reported the normal boiling temperature, Wilcock[12] reported the boiling temperature at normal pressure and 2.67 kPa (20 mmHg), Osthoff et al.[17] reported saturated vapor pressures in the range (343 to 388) K, Waterman et al.[15] reported the normal boiling temperature, Marsh[4] reported saturated vapor pressure in the range (298 to 333) K, Young [7] in the high-temperature range (505 to 586.5) K, Flaningam[18] in the range (362 to 460) K, and Ditsent et al.[25] in the range (334 to 448) K.

For DMCPS, Hurd[9] reported the normal boiling temperature, Fischer and Weiss[3] reported the boiling temperature at 100 kPa, and Flaningam[18] saturated vapor pressures in the range (384 to 496) K. Ditsent et al.[25] reported saturated vapor pressures in the range (365 to 483) K. At temperatures less that 380 K our data agreed with those of Ditsent et al.[25] for higher temperatures our saturated pressures are higher than those of Flaningam[18] and Ditsent et al.[25] There is systematic shift from 0 kPa at 380 K to 10 kPa at 480 K.

Densities and the liquid surface tension are interrelated by parachor.[20] The corresponding average values calculated using our data are 492.4 for HMCTS, 642.6 for OMCTS, and 799.7 for PMCPS all in $cm^3\cdot g^{1/4}\cdot s^{-1/2}\cdot mol^{-1}$ with constancy ± 2 $cm^3\cdot g^{1/4}\cdot s^{-1/2}\cdot mol.^{-1}$ Using these data we have introduced a new group ascribed to Si into the Quale's additive group contribution method as reported in Reid et al.[20] The estimated value of contribution is 29.5 $cm^3\cdot g^{1/4}\cdot s^{-1/2}\cdot mol.^{-1}$ Using this new contribution, the values of parachor have been predicted for 12 siloxanes (D3 to D7 and MM to MD6M) and for 1,1,1,3,3,3-hexamethyldisilazane and compared with the values taken from literature. For the "D series" the deviations were less than 1 %, except for D3. For D3 the deviation was 2.3 %, but D3 has particular structure and properties. For the "MD_nM series" the predicted values are lower than experimental, and the deviation has increased with the number of difunctional units from about 0 % for MM to 6.8 % for MD4M. For 1,1,1,3,3,3-hexamethyldisilazane the predicted value was higher of 4 %.

Elbro et al.[21] have proposed the group contribution method for the prediction of liquid densities as a function of temperature. This method contains the SiO group which together with the CH_3 group can be used for estimation of liquid densities in siloxanes. When applied to our data the corresponding rms deviations were equal to 77.8 $kg\cdot m^{-3}$ for HMCTS, 49.9 $kg\cdot m^{-3}$ for OMCTS, and 46.3 $kg\cdot m^{-3}$ for PMCPS. These deviations correspond to (22.4, 19.3, and 23.0) %, correspondingly. Recently Ihmels and Gmehling[22] revised and extended parameters reported by Elbro et al.[21] The new parameters results in better description of experimental data; the corresponding deviations are 63.2 $kg\cdot m^{-3}$ (18.6 %) for HMCTS, 34.6 $kg\cdot m^{-3}$ (14.0 %) for OMCTS, and 30.3 $kg\cdot m^{-3}$ (15.7 %) for PMCPS. The obtained deviation are smaller but still significant which perhaps results from particular structure of cyclic siloxanes. Therefore we have introduced a new group, designated as $SiO(CH_3)_2$, and estimated relevant parameters using data for OMCTS. The estimated group volume parameters are $A/cm^3\cdot mol^{-1} = 42.23$, $10^3B/cm^3\cdot mol^{-1}\cdot K^{-1} = 119.85$, and $10^5C/cm^3\cdot mol^{-1}\cdot K^{-2} = 0$. The resulting deviations were equal to 18.9 $kg\cdot m^{-3}$ (5.8 %) for HMCTS, 6.0 $kg\cdot m^{-3}$ (2.4 %) for OMCTS, and 14.6 $kg\cdot m^{-3}$ (7.7 %) for PMCPS, which compares favorably to Elbro et al.[21] and Ihmels and Gmehling.[22]

Conclusions

Liquid densities, viscosities, orthobaric heat capacities, surface tensions, thermal conductivities, and saturated vapor pressures were measured for a sample of 99.98 mol % pure HMCTS, OMCTS, and DMCPS over wide temperature ranges. To our knowledge, values for the liquid thermal conductivity for all the three siloxanes were for the first time measured and reported in this work. The experimental data were compared with available literature data.

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