Density, heat capacity and vapor pressure of squalane - supplementary material

Aleš Blahut[1*], Olga Prokopová[1], Václav Vinš[1], Vojtěch Štejfa[2], Lukas Soba[3], Monika Thol[3], Roland Span[3]

[1]Institute of Thermomechanics of the Czech Academy of Sciences, Dolejškova 1402/5, Praha 8, 182 00, Czech Republic.
[2]Department of Physical Chemistry, University of Chemistry and Technology, Prague, Technická 5, Prague 6, 166 28, Czech Republic.
[3]Chair of Thermodynamics, Ruhr University Bochum, Universitätsstraße 150, Bochum, 448 01, Germany.

*Corresponding author(s). E-mail(s): blahut@it.cas.cz;

S1. Experimental densities of squalane: single-sinker densimeter

Table S1: Experimental densities and their combined standard uncertainties for squalane obtained by the single-sinker densimeter. Data are tabulated in the chronological order.

$\frac{T^a}{K}$	$\frac{p}{\text{MPa}}$	$\frac{u_c(p)}{\text{MPa}}$	$\frac{\rho}{\text{kg m}^{-3}}$	$\frac{u_c(\rho)}{\text{kg m}^{-3}}$
293.153^b	0.1086	0.0004	808.145	0.028
293.154^b	0.1080	0.0004	808.142	0.028
293.154^b	0.1070	0.0004	808.141	0.028
293.153^b	0.1069	0.0004	808.141	0.028
293.148	19.9897	0.0090	819.191	0.029
293.150	20.0066	0.0101	819.197	0.029
293.150	20.0051	0.0091	819.197	0.029
293.150	19.9953	0.0115	819.192	0.029
293.153	15.0073	0.0034	816.560	0.028
293.152	15.0038	0.0026	816.556	0.028
293.151	15.0025	0.0024	816.557	0.028
293.150	14.9934	0.0027	816.551	0.028
293.154	9.9985	0.0017	813.825	0.028
293.153	9.9985	0.0018	813.828	0.028
293.152	10.0050	0.0010	813.831	0.028
293.149	5.0028	0.0014	811.002	0.028
293.149	5.0027	0.0024	811.004	0.028
293.148	5.0047	0.0017	811.003	0.028
293.155	0.9988	0.0007	808.658	0.028
293.154	0.9992	0.0005	808.656	0.028
293.153	1.0012	0.0011	808.658	0.028
293.153	1.0064	0.0009	808.661	0.028
293.154	0.1235	0.0037	808.133	0.028
293.153	0.1192	0.0026	808.132	0.028
293.152	0.1148	0.0020	808.130	0.028
293.151	0.1257	0.0015	808.137	0.028
298.147	19.9964	0.0024	816.235	0.028
298.147	19.9979	0.0024	816.237	0.028
298.149	19.9927	0.0027	816.233	0.028
298.150	14.9984	0.0028	813.540	0.028
298.149	15.0027	0.0024	813.543	0.028
298.150	14.9977	0.0024	813.541	0.028
298.149	10.0064	0.0009	810.758	0.028
298.149	10.0016	0.0009	810.755	0.028
298.150	10.0007	0.0012	810.755	0.028
298.149	5.0026	0.0015	807.862	0.028
298.150	5.0052	0.0011	807.864	0.028
298.151	5.0060	0.0009	807.864	0.028
298.151	1.0034	0.0008	805.468	0.028

(continued)

$\frac{T^a}{K}$	$\frac{p}{\text{MPa}}$	$\frac{u_c(p)}{\text{MPa}}$	$\frac{\rho}{\text{kg m}^{-3}}$	$\frac{u_c(\rho)}{\text{kg m}^{-3}}$
298.150	1.0017	0.0015	805.468	0.028
298.150	1.0029	0.0004	805.469	0.028
298.151	1.0031	0.0005	805.468	0.028
298.149	0.1172	0.0026	804.927	0.028
298.150	0.1159	0.0022	804.926	0.028
298.151	0.1143	0.0016	804.925	0.028
298.151	0.1113	0.0009	804.923	0.028
313.134	19.9978	0.0026	807.431	0.028
313.135	20.0022	0.0024	807.432	0.028
313.137	20.0063	0.0026	807.434	0.028
313.144	15.0041	0.0024	804.563	0.028
313.143	15.0029	0.0024	804.564	0.028
313.143	15.0030	0.0024	804.563	0.028
313.147	10.0090	0.0014	801.590	0.028
313.146	10.0024	0.0009	801.587	0.028
313.147	10.0029	0.0009	801.588	0.028
313.153	5.0065	0.0009	798.489	0.028
313.151	5.0009	0.0017	798.487	0.028
313.150	5.0029	0.0010	798.487	0.028
313.150	1.0052	0.0011	795.917	0.028
313.150	1.0092	0.0012	795.920	0.028
313.150	1.0048	0.0009	795.917	0.028
313.151	0.1115	0.0005	795.324	0.028
313.151	0.1142	0.0005	795.326	0.028
313.151	0.1159	0.0004	795.327	0.028
313.150	0.1253	0.0004	795.335	0.028
313.151	0.1262	0.0004	795.334	0.028
333.156	20.0043	0.0024	795.789	0.028
333.155	20.0039	0.0024	795.790	0.028
333.155	20.0042	0.0024	795.790	0.028
333.155	15.0000	0.0024	792.676	0.028
333.153	15.0047	0.0025	792.679	0.028
333.152	15.0062	0.0024	792.681	0.028
333.153	10.0027	0.0016	789.437	0.028
333.151	10.0031	0.0009	789.438	0.028
333.151	10.0054	0.0009	789.440	0.028
333.154	5.0029	0.0010	786.047	0.028
333.153	5.0028	0.0009	786.047	0.028
333.152	5.0030	0.0009	786.048	0.028
333.154	1.0107	0.0014	783.224	0.028
333.152	1.0085	0.0015	783.225	0.028
333.151	1.0054	0.0019	783.223	0.028
333.151	1.0053	0.0012	783.223	0.028
333.151	1.0122	0.0013	783.228	0.028

(continued)

$\frac{T^a}{K}$	$\frac{p}{\text{MPa}}$	$\frac{u_c(p)}{\text{MPa}}$	$\frac{\rho}{\text{kg m}^{-3}}$	$\frac{u_c(\rho)}{\text{kg m}^{-3}}$
333.152	0.1270	0.0011	782.588	0.028
333.151	0.1191	0.0009	782.582	0.028
333.150	0.1225	0.0024	782.584	0.028
353.154	19.9965	0.0031	784.293	0.028
353.155	20.0095	0.0026	784.300	0.028
353.154	20.0206	0.0039	784.308	0.028
353.151	14.9953	0.0035	780.921	0.028
353.151	14.9928	0.0035	780.921	0.028
353.151	14.9937	0.0037	780.921	0.028
353.153	10.0222	0.0061	777.403	0.028
353.151	10.0277	0.0051	777.408	0.028
353.150	10.0154	0.0034	777.401	0.028
353.151	10.0146	0.0025	777.399	0.028
353.152	5.0003	0.0011	773.677	0.027
353.151	4.9981	0.0010	773.676	0.027
353.150	4.9991	0.0009	773.678	0.027
353.153	1.0172	0.0035	770.577	0.028
353.151	1.0093	0.0010	770.573	0.028
353.150	1.0004	0.0013	770.566	0.028
353.151	0.1290	0.0025	769.869	0.028
353.150	0.1274	0.0020	769.869	0.028
353.150	0.1391	0.0015	769.878	0.028
373.151	20.0108	0.0025	772.930	0.027
373.150	20.0007	0.0025	772.924	0.027
373.151	20.0056	0.0025	772.926	0.027
373.149	15.0057	0.0024	769.263	0.027
373.150	15.0041	0.0025	769.263	0.027
373.152	15.0000	0.0027	769.257	0.027
373.154	10.0075	0.0009	765.409	0.027
373.154	10.0064	0.0010	765.409	0.027
373.154	10.0102	0.0012	765.412	0.027
373.150	5.0145	0.0020	761.353	0.027
373.151	5.0096	0.0014	761.347	0.027
373.153	5.0042	0.0009	761.342	0.027
373.156	1.0035	0.0004	757.910	0.027
373.155	1.0025	0.0004	757.910	0.027
373.154	1.0017	0.0005	757.911	0.027
373.155	0.1197	0.0019	757.129	0.027
373.155	0.1230	0.0020	757.133	0.027
373.154	0.1191	0.0018	757.130	0.027
393.148	20.0068	0.0026	761.653	0.027
393.150	20.0090	0.0024	761.655	0.027
393.152	19.9997	0.0025	761.648	0.027
393.154	14.9973	0.0027	757.669	0.027

(continued)

$\frac{T^a}{K}$	$\frac{p}{\text{MPa}}$	$\frac{u_c(p)}{\text{MPa}}$	$\frac{\rho}{\text{kg m}^{-3}}$	$\frac{u_c(\rho)}{\text{kg m}^{-3}}$
393.152	14.9990	0.0026	757.673	0.027
393.150	15.0005	0.0031	757.675	0.027
393.153	10.0049	0.0014	753.479	0.027
393.153	10.0079	0.0009	753.483	0.027
393.152	10.0100	0.0009	753.485	0.027
393.156	5.0075	0.0009	749.022	0.027
393.156	5.0038	0.0010	749.018	0.027
393.154	1.0050	0.0006	745.240	0.027
393.154	1.0111	0.0006	745.246	0.027
393.150	0.1245	0.0023	744.381	0.027
393.150	0.1215	0.0019	744.378	0.027
413.152	20.0043	0.0024	750.466	0.027
413.153	20.0081	0.0025	750.469	0.027
413.153	15.0042	0.0024	746.158	0.027
413.151	15.0026	0.0024	746.159	0.027
413.149	10.0113	0.0010	741.591	0.027
413.148	10.0072	0.0011	741.588	0.027
413.148	10.0211	0.0027	741.600	0.027
413.154	5.0096	0.0012	736.697	0.027
413.153	4.9978	0.0013	736.686	0.027
413.152	5.0059	0.0012	736.695	0.027
413.151	1.0053	0.0010	732.517	0.027
413.151	1.0174	0.0019	732.530	0.027
413.151	0.1229	0.0022	731.559	0.027
413.150	0.1155	0.0015	731.552	0.027
433.155	19.9990	0.0029	739.352	0.027
433.154	19.9992	0.0034	739.352	0.027
433.154	15.0027	0.0024	734.687	0.027
433.153	14.9991	0.0025	734.684	0.027
433.152	10.0095	0.0009	729.707	0.027
433.150	10.0071	0.0009	729.705	0.027
433.150	10.0022	0.0010	729.700	0.027
433.151	5.0066	0.0009	724.335	0.027
433.150	5.0061	0.0011	724.335	0.027
433.150	1.0020	0.0007	719.708	0.027
433.150	1.0031	0.0007	719.709	0.027
433.150	1.0027	0.0005	719.708	0.027
433.151	0.1274	0.0020	718.652	0.027
433.151	0.1193	0.0006	718.643	0.027
433.151	0.1224	0.0006	718.646	0.027
453.153	20.0103	0.0027	728.327	0.027
453.151	20.0049	0.0026	728.323	0.027
453.150	19.9975	0.0025	728.316	0.027
453.152	15.0025	0.0026	723.261	0.027

(continued)

$\frac{T^a}{K}$	$\frac{p}{\text{MPa}}$	$\frac{u_c(p)}{\text{MPa}}$	$\frac{\rho}{\text{kg m}^{-3}}$	$\frac{u_c(\rho)}{\text{kg m}^{-3}}$
453.151	14.9994	0.0025	723.259	0.027
453.150	10.0053	0.0011	717.826	0.027
453.150	10.0072	0.0010	717.828	0.027
453.150	5.0087	0.0012	711.929	0.027
453.150	5.0076	0.0012	711.926	0.027
453.150	5.0071	0.0009	711.927	0.027
453.151	1.0035	0.0005	706.799	0.027
453.150	1.0054	0.0005	706.801	0.027
453.152	0.1282	0.0014	705.619	0.027
453.152	0.1230	0.0011	705.614	0.027
453.152	0.1234	0.0012	705.614	0.027
293.153[b]	20.0087	0.0027	819.183	0.028
293.152[b]	20.0048	0.0024	819.180	0.028
293.152[b]	20.0026	0.0024	819.180	0.028
293.153[b]	15.0063	0.0024	816.543	0.028
293.153[b]	14.9998	0.0032	816.539	0.028
293.153[b]	15.0014	0.0027	816.540	0.028
293.151[b]	10.0172	0.0018	813.821	0.028
293.151[b]	10.0016	0.0010	813.813	0.028
293.153[b]	5.0064	0.0012	810.986	0.028
293.151[b]	5.0135	0.0016	810.991	0.028
293.153[b]	1.0107	0.0013	808.649	0.028
293.152[b]	1.0032	0.0005	808.645	0.028
293.151[b]	1.0064	0.0018	808.647	0.028
293.151[b]	0.1239	0.0033	808.119	0.028
293.151[b]	0.1187	0.0007	808.117	0.028
293.152[b]	0.1223	0.0005	808.119	0.028
293.152[b]	0.1258	0.0006	808.122	0.028
293.153[b]	0.1287	0.0007	808.124	0.028

[a] The combined standard uncertainty of temperature is $u_c(T) = 0.02\,\text{K}$.
[b] Check measurements, data were not used for the development of density correlations.

Table S2: Example of the uncertainty budget for the single-sinker density measurement, $T = 373.154\,\mathrm{K}$, $p = 10.0064\,\mathrm{MPa}$

Source of uncertainty	Uncertainty $u(x_i)$	Distribution	Sensitivity coefficient c_i	Uncertainty contribution $u_i(\mathrm{kg\,m^{-3}})$
Density measurement				0.0195
Weighing in fluid	3.90×10^{-5} g	normal	$-5.32 \times 10^{1}\,\mathrm{kg\,m^{-3}\,g^{-1}}$	−0.0021
Weighing in vacuum	5.67×10^{-5} g	normal	$5.32 \times 10^{1}\,\mathrm{kg\,m^{-3}\,g^{-1}}$	0.0030
Sinker volume at ref. cond.	$3.61 \times 10^{-4}\,\mathrm{cm^3}$	normal	$-4.07 \times 10^{1}\,\mathrm{kg\,m^{-3}\,cm^{-3}}$	−0.0147
Sinker volume drift	$4.29 \times 10^{-4}\,\mathrm{cm^3}$	rectangular	$-4.07 \times 10^{1}\,\mathrm{kg\,m^{-3}\,cm^{-3}}$	−0.0101
Sinker T−correction	$9.19 \times 10^{-3}\,\mathrm{kg\,m^{-3}}$	rectangular	1	0.0053
Sinker p−correction	$7.81 \times 10^{-4}\,\mathrm{kg\,m^{-3}}$	rectangular	1	0.0005
Buoyancy correction	$5.49 \times 10^{-3}\,\mathrm{kg\,m^{-3}}$	rectangular	1	0.0032
Force-transmission error	$5.50 \times 10^{-3}\,\mathrm{kg\,m^{-3}}$	rectangular	1	0.0032
Temperature measurement				0.0115
Calibration of thermometer	4.00×10^{-3} K	normal	$-6.03 \times 10^{-1}\,\mathrm{kg\,m^{-3}\,K^{-1}}$	−0.0024
Calibration of std. resistor	4.00×10^{-3} K	normal	$-6.03 \times 10^{-1}\,\mathrm{kg\,m^{-3}\,K^{-1}}$	−0.0024
Thermometer drift	1.00×10^{-2} K	rectangular	$-6.03 \times 10^{-1}\,\mathrm{kg\,m^{-3}\,K^{-1}}$	−0.0035
Drift of standard resistor	2.00×10^{-3} K	rectangular	$-6.03 \times 10^{-1}\,\mathrm{kg\,m^{-3}\,K^{-1}}$	−0.0007
Temperature uniformity	3.00×10^{-2} K	rectangular	$-6.03 \times 10^{-1}\,\mathrm{kg\,m^{-3}\,K^{-1}}$	−0.0104
Temperature stability	1.38×10^{-4} K	rectangular	$-6.03 \times 10^{-1}\,\mathrm{kg\,m^{-3}\,K^{-1}}$	−0.0000
Pressure measurement				0.0007
Pressure transducer	1.38×10^{-3} MPa	rectangular	$7.57 \times 10^{-1}\,\mathrm{kg\,m^{-3}\,MPa^{-1}}$	0.0006
Diff. pressure sensor	1.75×10^{-4} MPa	rectangular	$7.57 \times 10^{-1}\,\mathrm{kg\,m^{-3}\,MPa^{-1}}$	0.0001
p_{hyd} correction	4.74×10^{-4} MPa	rectangular	$7.57 \times 10^{-1}\,\mathrm{kg\,m^{-3}\,MPa^{-1}}$	0.0002
Pressure stability	8.73×10^{-4} MPa	rectangular	$7.57 \times 10^{-1}\,\mathrm{kg\,m^{-3}\,MPa^{-1}}$	0.0004
Repeatability[a]	$1.53 \times 10^{-2}\,\mathrm{kg\,m^{-3}}$	normal	1	0.0153
$\rho\,(373.154\,\mathrm{K},\ 10.0064\,\mathrm{MPa}) = 765.4088\,\mathrm{kg\,m^{-3}}$				0.0274

[a] The estimate is based on check measurements performed at 293.15 K.

S2. Density correlations - deviation plots

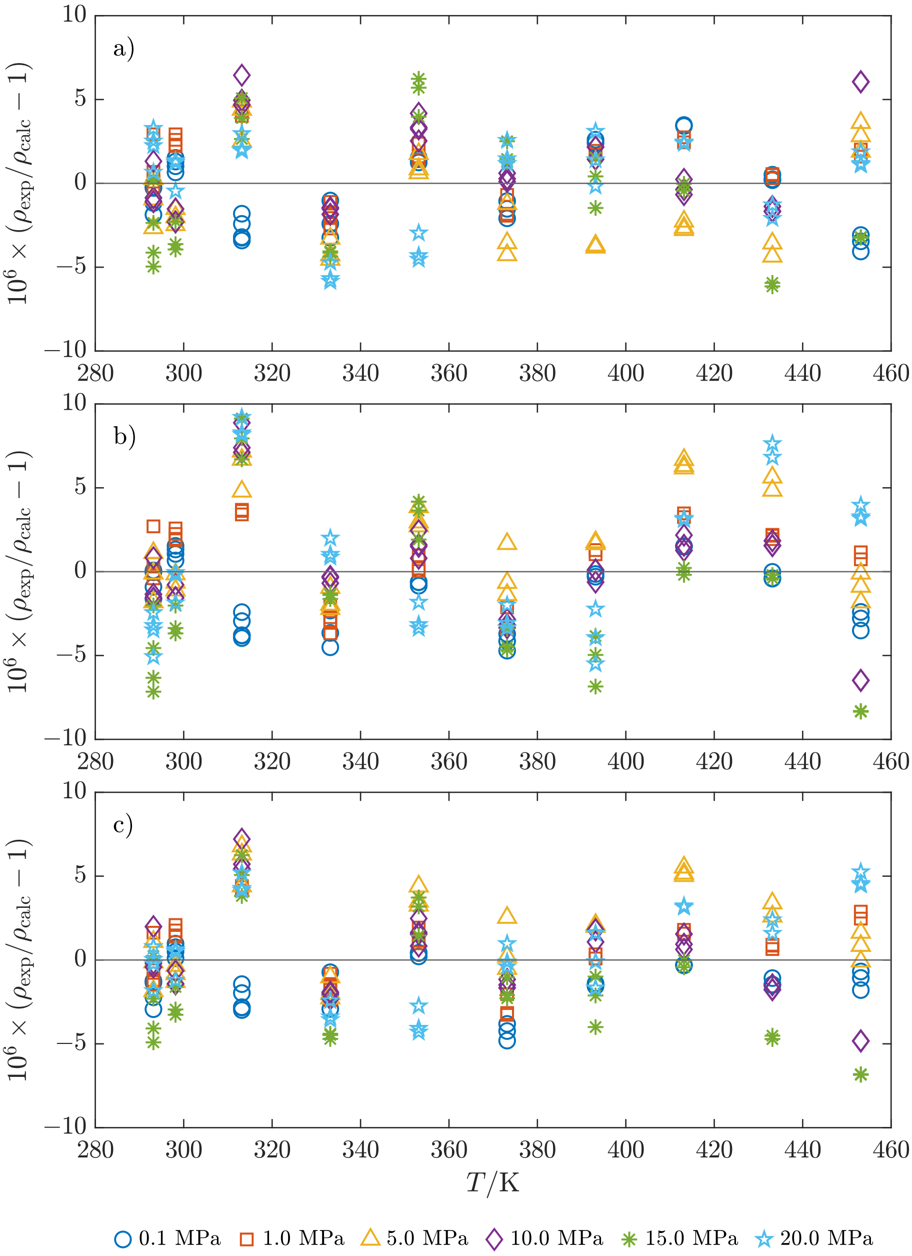

Fig. S1: Relative deviations of the single-sinker densities from densities calculated using different correlations: a) the seven-term correlation, b) the modified Tait equation with $B = b_3 T_r^3 + b_2 T_r^2 + b_1 T_r + b_0$, c) the modified Tait equation with $B = b_2 T_r + b_1 T_r^{0.03} + b_0$

S3. Isobaric expansivity and isothermal compressibility graphs

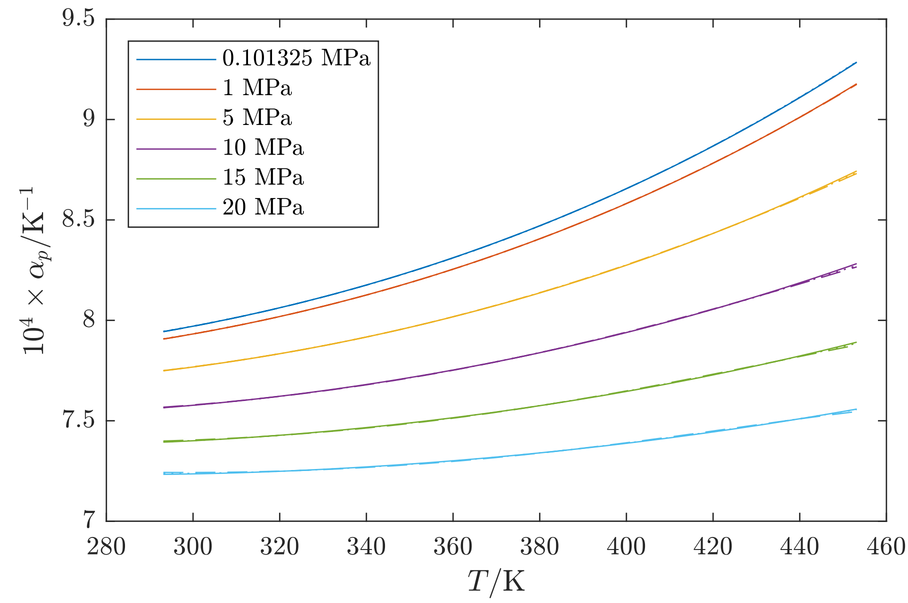

Fig. S2: Isobaric expansivity of squalane, α_p, calculated using developed density correlations: the seven-term correlation (solid line), the modified Tait equation with $B = b_3 T_\mathrm{r}^3 + b_2 T_\mathrm{r}^2 + b_1 T_\mathrm{r} + b_0$ (dashed line), the modified Tait equation with $B = b_2 T_\mathrm{r} + b_1 T_\mathrm{r}^{0.03} + b_0$ (dotted line)

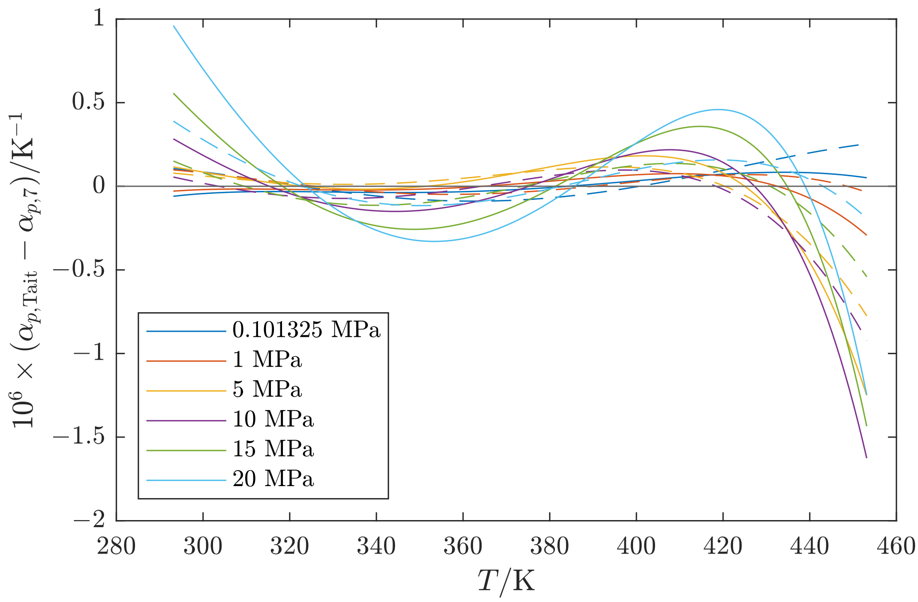

Fig. S3: Deviations of isobaric expansivity, α_p, calculated using the modified Tait equation and the seven-term equation: the modified Tait equation with $B = b_3 T_\mathrm{r}^3 + b_2 T_\mathrm{r}^2 + b_1 T_\mathrm{r} + b_0$ (solid line), the modified Tait equation with $B = b_2 T_\mathrm{r} + b_1 T_\mathrm{r}^{0.03} + b_0$ (dashed line)

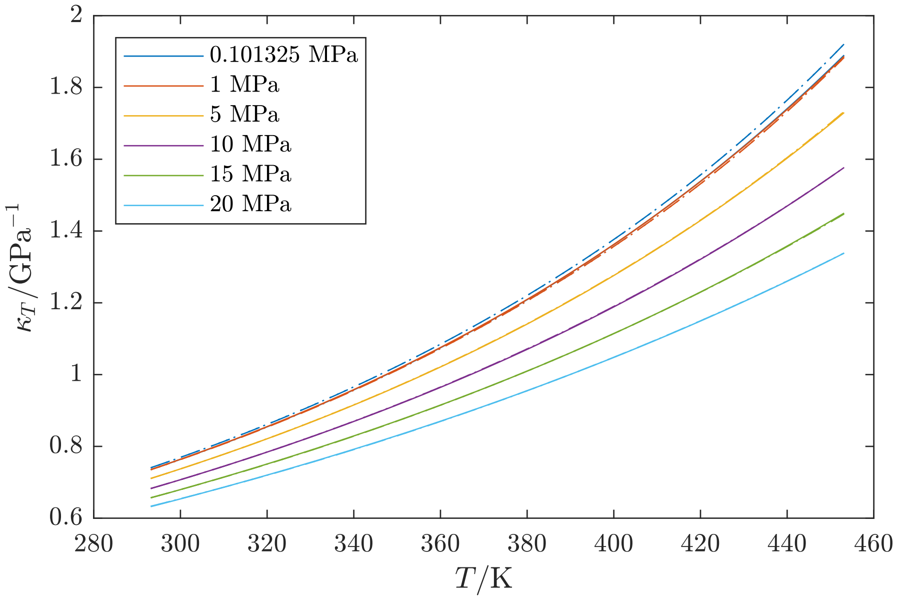

Fig. S4: Isothermal compressibility of squalane, κ_T, calculated using developed density correlations: seven-term correlation (solid line), the modified Tait equation with $B = b_3\,T_\mathrm{r}^3 + b_2\,T_\mathrm{r}^2 + b_1\,T_\mathrm{r} + b_0$ (dashed line), the modified Tait equation with $B = b_2\,T_\mathrm{r} + b_1\,T_\mathrm{r}^{0.03} + b_0$ (dotted line)

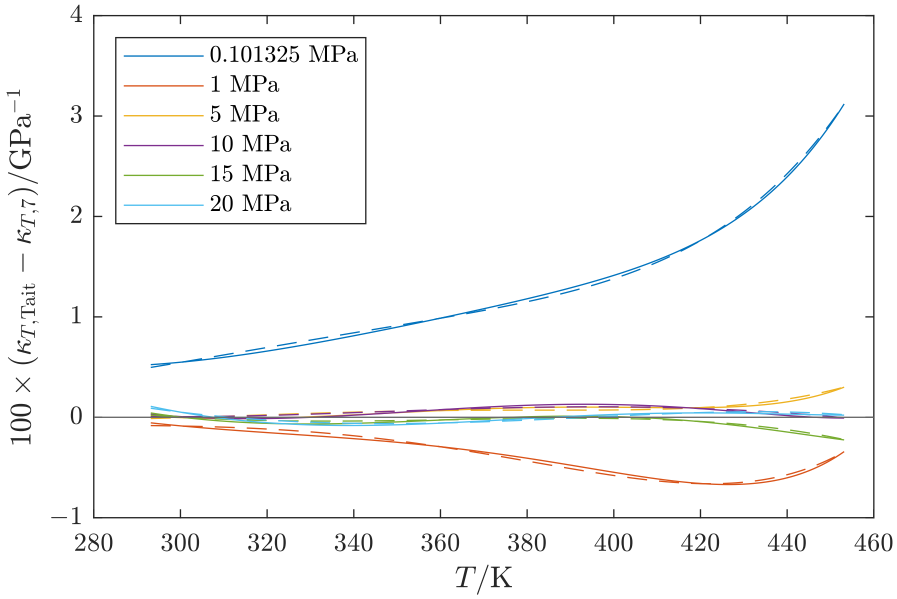

Fig. S5: Deviations of isothermal compressibility, κ_T, calculated using the modified Tait equation and the seven-term equation: the modified Tait equation with $B = b_3\,T_\mathrm{r}^3 + b_2\,T_\mathrm{r}^2 + b_1\,T_\mathrm{r} + b_0$ (solid line), the modified Tait equation with $B = b_2\,T_\mathrm{r} + b_1\,T_\mathrm{r}^{0.03} + b_0$ (dashed line)

S4. Estimation of ideal-gas heat capacities

Table S3: Ideal-gas heat capacity $C^\circ_{p,\mathrm{m}}/\left(\mathrm{J\,K^{-1}\,mol^{-1}}\right)$ estimated using the modified Benson [1], the modified Joback [2], and the Coniglio and Daridon [3] group contribution methods

T/K	Method		
	Mod. Benson[a]	Mod. Joback	Coniglio and Daridon[b]
260	615	613	603
280	654	657	648
300	693	700	691
320	731	741	733
340	769	782	774
360	806	822	815
380	843	860	854
400	879	897	892
420	914	933	928
440	948	969	964
460	981	1003	998
480	1014	1036	1031
500	1046	1068	1062
520	1076	1099	1093
540	1106	1129	1122
560	1135	1159	1150
580	1163	1187	1177
600	1190	1215	1202

[a] Values below 300 K are extrapolated.

[b] $C^\circ_{p,\mathrm{m}}$ values obtained using the method of Coniglio and Daridon were used in simultaneous correlation within the development of vapor pressure equation for squalane. Expanded uncertainty (k = 2) of the ideal-gas heat capacities is estimated to be $U\left(C^\circ_{p,\mathrm{m}}\right) = 0.03 \times C^\circ_{p,\mathrm{m}}$.

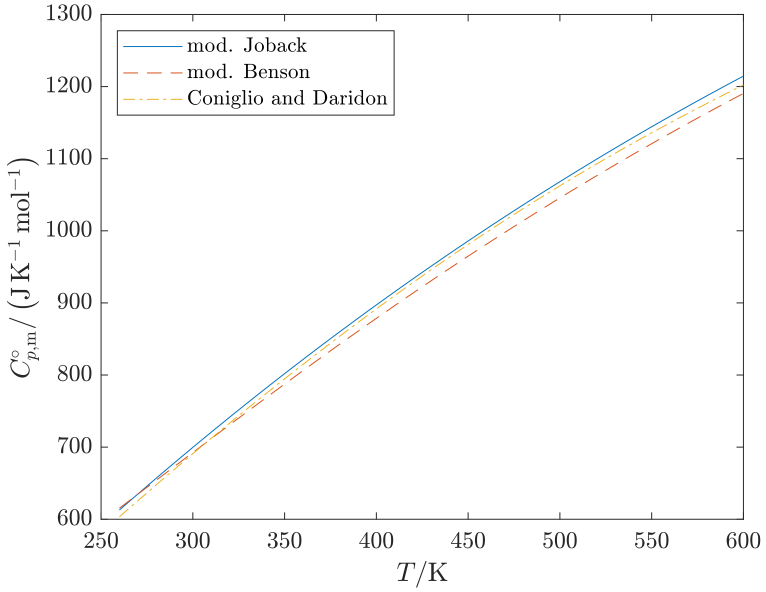

Fig. S6: Comparison of the ideal-gas heat capacities for squalane obtained by the modified Benson [1], the modified Joback [2], and the Coniglio and Daridon [3] group contribution methods

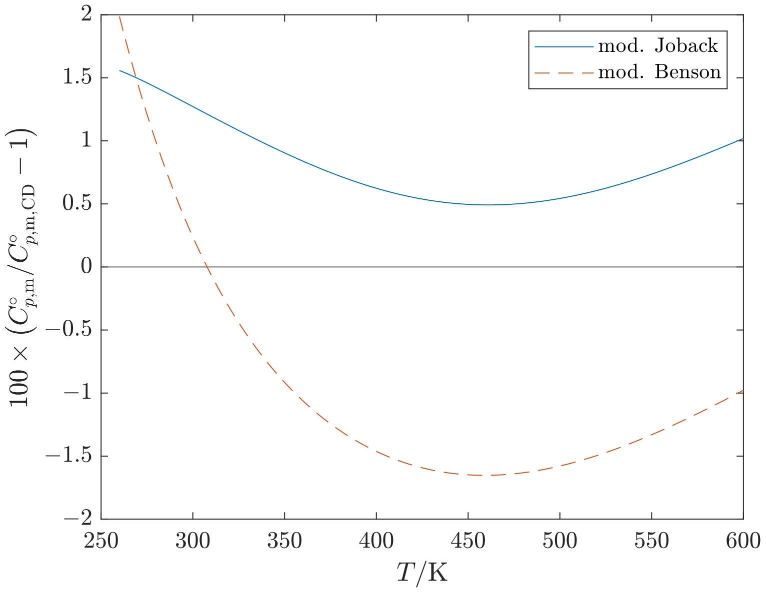

Fig. S7: Percent relative deviations of the ideal-gas heat capacities for squalane estimated by the modified Benson [1] and the modified Joback [2] methods from those calculated with the method of Coniglio and Daridon [3]

S5. Vapor pressures and vaporization thermodynamic functions of squalane

Table S4: Values of saturated vapor pressure and vaporization thermodynamic functions of squalane based on the Wagner equation (for details, see the main article). Expanded uncertainties, $U(k = 2)$, of the associated properties were determined using the Monte Carlo method and the error propagation law.

$\frac{T}{\mathrm{K}}$	$\frac{p}{\mathrm{Pa}}$	$\frac{U(p)}{\mathrm{Pa}}$	$\frac{W^a}{\mathrm{kJ\,mol^{-1}}}$	$\frac{U(W)}{\mathrm{kJ\,mol^{-1}}}$	$\frac{\Delta_l^g H_m}{\mathrm{kJ\,mol^{-1}}}$	$\frac{U(\Delta_l^g H_m)}{\mathrm{kJ\,mol^{-1}}}$	$\frac{\mathrm{d}W/\mathrm{d}T}{\mathrm{J\,K^{-1}\,mol^{-1}}}$	$\frac{U(\mathrm{d}W/\mathrm{d}T)}{\mathrm{J\,K^{-1}\,mol^{-1}}}$	$\frac{\Delta_l^g C_{p,m}^\circ}{\mathrm{J\,K^{-1}\,mol^{-1}}}$	$\frac{U(\Delta_l^g C_{p,m}^\circ)}{\mathrm{J\,K^{-1}\,mol^{-1}}}$
260	714×10^{-12}	188×10^{-12}	139.3	3.7	139.3	3.7	−220.2	41.5	−220.2	41.5
270	7.63×10^{-9}	1.78×10^{-9}	137.2	3.6	137.2	3.6	−215.2	35.5	−215.2	35.5
280	66.5×10^{-9}	13.8×10^{-9}	135.0	3.5	135.0	3.5	−210.5	30.2	−210.5	30.2
290	484×10^{-9}	88×10^{-9}	133.0	3.4	133.0	3.4	−206.1	25.9	−206.1	25.9
298.15	2.17×10^{-6}	0.35×10^{-6}	131.3	3.4	131.3	3.4	−202.8	23.1	−202.8	23.1
300	3.00×10^{-6}	0.48×10^{-6}	130.9	3.4	130.9	3.4	−202.0	22.5	−202.0	22.5
310	16.1×10^{-6}	2.2×10^{-6}	128.9	3.3	128.9	3.3	−198.3	20.2	−198.3	20.2
320	76.0×10^{-6}	9.1×10^{-6}	127.0	3.2	127.0	3.2	−194.8	18.8	−194.8	18.8
330	319×10^{-6}	33×10^{-6}	125.0	3.0	125.0	3.0	−191.5	18.4	−191.5	18.4
340	1.21×10^{-3}	0.1×10^{-3}	123.1	2.9	123.1	2.9	−188.5	18.6	−188.5	18.6
350	4.15×10^{-3}	0.3×10^{-3}	121.3	2.7	121.3	2.7	−185.7	19.2	−185.7	19.2
360	13.1×10^{-3}	0.8×10^{-3}	119.4	2.6	119.4	2.6	−183.1	20.0	−183.1	20.0
370	38.2×10^{-3}	1.9×10^{-3}	117.6	2.4	117.6	2.4	−180.6	20.9	−180.6	20.9
380	104×10^{-3}	4×10^{-3}	115.8	2.2	115.8	2.2	−178.2	21.7	−178.2	21.7
390	263×10^{-3}	8×10^{-3}	114.0	2.1	114.0	2.1	−175.9	22.4	−175.9	22.4
400	630×10^{-3}	15×10^{-3}	112.3	1.9	112.3	1.9	−173.6	22.9	−173.7	22.9
410	1.425	0.026	110.6	1.7	110.6	1.7	−171.3	23.2	−171.5	23.3
420	3.067	0.040	108.9	1.5	108.8	1.5	−169.1	23.3	−169.3	23.5
430	6.296	0.056	107.2	1.4	107.2	1.4	−166.8	23.3	−167.2	23.5

(continued)

$\frac{T}{\mathrm{K}}$	$\frac{p}{\mathrm{Pa}}$	$\frac{U(p)}{\mathrm{Pa}}$	$\frac{W^{a}}{\mathrm{kJ\,mol^{-1}}}$	$\frac{U(W)}{\mathrm{kJ\,mol^{-1}}}$	$\frac{\Delta_{\mathrm{l}}^{\mathrm{g}}H_{\mathrm{m}}}{\mathrm{kJ\,mol^{-1}}}$	$\frac{U(\Delta_{\mathrm{l}}^{\mathrm{g}}H_{\mathrm{m}})}{\mathrm{kJ\,mol^{-1}}}$	$\frac{\mathrm{d}W/\mathrm{d}T}{\mathrm{J\,K^{-1}\,mol^{-1}}}$	$\frac{U(\mathrm{d}W/\mathrm{d}T)}{\mathrm{J\,K^{-1}\,mol^{-1}}}$	$\frac{\Delta_{\mathrm{l}}^{\mathrm{g}}C_{p,\mathrm{m}}^{\circ}}{\mathrm{J\,K^{-1}\,mol^{-1}}}$	$\frac{U(\Delta_{\mathrm{l}}^{\mathrm{g}}C_{p,\mathrm{m}}^{\circ})}{\mathrm{J\,K^{-1}\,mol^{-1}}}$
440	12.38	0.07	105.5	1.3	105.5	1.3	−164.5	23.0	−165.1	23.3
450	23.38	0.12	103.9	1.2	103.9	1.2	−162.1	22.6	−163.0	23.1
460	42.56	0.27	102.3	1.1	102.2	1.2	−159.6	22.1	−160.9	22.7
470	74.85	0.64	100.7	1.1	100.6	1.2	−157.0	21.4	−158.9	22.3
480	127.5	1.4	99.1	1.2	99.0	1.2	−154.3	20.5	−156.9	21.7
490	210.9	2.9	97.6	1.2	97.5	1.3	−151.4	19.4	−155.0	21.2
500	339.3	5.5	96.1	1.3	95.9	1.4	−148.3	18.3	−153.1	20.6
510	532.0	10.0	94.6	1.4	94.4	1.5	−145.1	17.0	−151.3	20.0
520	814.5	17.4	93.2	1.4	92.9	1.6	−141.7	15.7	−149.6	19.4
530	1220	29	91.8	1.5	91.3	1.7	−138.1	14.2	−147.9	18.8
540	1789	48	90.4	1.6	89.8	1.9	−134.2	12.8	−146.3	18.5
550	2573	76	89.1	1.7	88.3	2.0	−130.2	11.3	−144.7	18.3
560	3635	118	87.8	1.7	86.8	2.1	−125.9	10.0	−143.1	18.5
570	5049	178	86.6	1.7	85.3	2.3	−121.3	9.0	−141.5	19.4
580	6904	261	85.4	1.8	83.8	2.4	−116.6	8.5	−139.8	21.3
590	9303	376	84.3	1.7	82.3	2.5	−111.5	8.6	−138.1	24.1
600	12365	531	83.2	1.7	80.8	2.7	−106.2	9.7	−136.1	27.8
610	16225	734	82.2	1.7			−100.6	11.3		
620	21036	995	81.2	1.6			−94.7	13.7		
630	26971	1327	80.3	1.5			−88.5	16.4		
640	34223	1738	79.4	1.3			−82.0	19.6		
650	43006	2240	78.6	1.2			−75.1	23.0		
660	53557	2842	77.9	1.0			−67.9	26.9		

(continued)

$\frac{T}{\mathrm{K}}$	$\frac{p}{\mathrm{Pa}}$	$\frac{U(p)}{\mathrm{Pa}}$	$\frac{W^a}{\mathrm{kJ\,mol^{-1}}}$	$\frac{U(W)}{\mathrm{kJ\,mol^{-1}}}$	$\frac{\Delta_l^g H_m}{\mathrm{kJ\,mol^{-1}}}$	$\frac{U(\Delta_l^g H_m)}{\mathrm{kJ\,mol^{-1}}}$	$\frac{\mathrm{d}W/\mathrm{d}T}{\mathrm{J\,K^{-1}\,mol^{-1}}}$	$\frac{U(\mathrm{d}W/\mathrm{d}T)}{\mathrm{J\,K^{-1}\,mol^{-1}}}$	$\frac{\Delta_l^g C_{p,m}^\circ}{\mathrm{J\,K^{-1}\,mol^{-1}}}$	$\frac{U(\Delta_l^g C_{p,m}^\circ)}{\mathrm{J\,K^{-1}\,mol^{-1}}}$
670	66140	3550	77.3	0.9			−60.3	31.1		
680	81043	4365	76.7	0.8			−52.3	35.6		
690	98590	5286	76.2	0.8			−43.8	40.7		
700	119136	6301	75.8	1.1			−34.9	46.3		
710	143077	7388	75.5	1.4			−25.3	54.3		
720	170856	8512	75.3	1.9			−15.0	62.3		
730	202970	9618	75.2	2.5			−3.9	70.3		
740	239980	10627	75.3	3.2			8.3	78.3		
750	282524	11425	75.4	4.0			21.9	86.3		
760	331339	11854	75.7	4.9			37.6	94.3		
770	387284	11694	76.2	6.0			56.6	102.3		
780	451383	13542	76.8	7.3			82	110		
790	524904	15747	77.8	9.0			122	118		
800	609562	18287	79.5	11.6			232	126		

[a] $W = RT^2 \mathrm{d}\ln p/\mathrm{d}T = \Delta_l^g H_m/\Delta_l^g Z$ is the Waring function, which converges to the vaporization enthalpy $\Delta_l^g H_m$ at low vapor pressures.

S6. Parameters of the Wagner equation

Two forms of the following Wagner equation were considered for the simultaneous correlation of squalane vapor pressures

$$\ln \frac{p}{p_\mathrm{c}} = \frac{T_\mathrm{c}}{T}\left(A\,\tau + B\,\tau^{1.5} + C\,\tau^{c} + D\,\tau^{d}\right), \tag{1}$$

where p_c and T_c are the critical pressure and temperature, respectively, $\tau = 1 - T/T_\mathrm{c}$, and A, B, C, and D are the adjustable parameters.

Results for two forms labeled as 3–6 (c = 3, d = 6) and 3–10 (c = 3, d = 10) are compared in Table S5.

Table S5: Parameters of the Wagner equation for saturated vapor pressures of liquid squalane valid in the temperature range from 260 K to 805 K. Comparison of results for 3–6 and 3–10 forms of the Wagner equation.

Eq. form	T_c (K)	p_c (Pa)	A	B	C	D	σ_r[a] (%)	AARD(p)[b] (%)	AARD($\Delta_\mathrm{l}^\mathrm{g} C_{p,\mathrm{m}}^\circ$)[c] (%)
3–6	805	657000	−11.89008	2.12416	−12.51428	−4.27393	1.90	1.41	4.46
3–10	805	657000	−12.22707	3.00321	−14.12809	−6.88670	1.94	1.41	2.20

[a] σ_r is the relative standard deviation of the fit defined as $\sigma_\mathrm{r} = \sqrt{\sum_{i=1}^{n} (\Delta \ln p)_i^2/(n-m)}$, where $\Delta \ln p$ is the difference between the logarithm of the experimental and the smoothed vapor pressure values, n is the number of experimental points used in the fit, and m is the number of adjustable parameters of the Wagner equation.

[b] Average absolute relative deviation between calculated and experimental vapor pressures involved in the simultaneous correlation.

[c] Average absolute relative deviation between calculated and experimental values of heat capacity differences $\Delta_\mathrm{l}^\mathrm{g} C_{p,\mathrm{m}}^\circ$ involved in the simultaneous correlation.

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