Supporting Information

Thermophysical property modelling of lubricant oils and their mixtures with refrigerants using a minimal set of experimental data

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S1. Models

S1.1 Raoult's law of boiling point elevation

At a certain pressure, for a pure solvent with a mass m_{solvent}, the boiling temperature is fixed at T_{solvent}. Added with a small mass of solute m_{solute} (for example m_{solute} / m_{solvent} = 0.02), the boiling temperature of the solution at the same pressure becomes T_{solution}. Then the molality b_{solute} of solute can be calculated with:

$$b_{\text{solute}} = (T_{\text{solution}} - T_{\text{solvent}})/K_{\text{b}} \quad \text{(S1)}$$

Here, K_{b} is a boiling point elevation constant, which is determined by the solvent and pressure, and is independent to the solute. Then the mole n_{solute} and molar mass M_{solute} of the solute can be calculate with:

$$n_{\text{solute}} = b_{\text{solute}} \cdot m_{\text{solvent}} \quad \text{(S2)}$$

$$M_{\text{solute}} = m_{\text{solute}}/n_{\text{solute}} \quad \text{(S3)}$$

S1.2 Modified Rackett Equation

A original Rackett equation [1,2] can be formulated as:

$$\rho_{\mathrm{sat,\,L}} = \rho_{\mathrm{c}} Z_{\mathrm{c}}^{-(1-T/T_{\mathrm{c}})^{2/7}} \tag{S4}$$

where $\rho_{\mathrm{sat,L}}$ is saturated liquid density, ρ_{c} ,T_{c} and Z_{c} are density, temperature, and compressibility factor at the critical point respectively, and T is temperature. For a lubricant, $\rho_{\mathrm{sat,L}}$ is very difficult to measure as the saturated pressure is very low (typically less than 1.0 Pa). Considering that, far away from the critical point, liquid density is insensitive to pressure, we here propose a modified Rackett equation:

$$\rho_{\mathrm{atm}} = \rho_{\mathrm{c}} Z_{\mathrm{c}}^{-(1-T/T_{\mathrm{c}})^{2/7}} \tag{S5}$$

in which, liquid density ρ_{atm} at atmosphere pressure (p_{atm} = 0.1 MPa) is used instead of $\rho_{\mathrm{sat,L}}$.

S1.3 Generalized three-parameter cubic EoS

The generalized three-parameter cubic equation of state (EoS) is formulated as follows [3,4]:

$$p = \frac{RT}{v - b_{\mathrm{m}}} - \frac{a_{\mathrm{m}}}{v^2 + (b_{\mathrm{m}} + c_{\mathrm{m}})v - b_{\mathrm{m}}c_{\mathrm{m}}} \tag{S6}$$

Here p is the pressure, R = 8.3144598 J·K^{-1}·mol^{-1} is the gas constant, and v is the molar volume. The subscript 'm' denotes mixtures, remove which, Eq. (S6) is for pure fluids. For pure and quasi-pure fluids, the parameters a, b and c are calculated as follows:

$$a = \alpha(T_r,\omega)\cdot\Omega_{\mathrm{a}}\frac{R^2T_{\mathrm{c}}^2}{p_{\mathrm{c}}} \tag{S7}$$

$$b = \Omega_{\mathrm{b}}\frac{RT_{\mathrm{c}}}{p_{\mathrm{c}}} \tag{S8}$$

$$c = \Omega_{\mathrm{c}}\frac{RT_{\mathrm{c}}}{p_{\mathrm{c}}} \tag{S9}$$

Here $T_{\mathrm{r}} = T/T_{\mathrm{c}}$ is the reduced temperature, while T_{c}, p_{c} and ω are the critical temperature, critical pressure, and acentric factor respectively. The function $\alpha(T_{\mathrm{r}}, \omega)$ and the parameters Ω_{a}, Ω_{b} and Ω_{c} are specifically formulated for each EoS, see details in Table S1. For mixtures, parameters a_{m}, b_{m} and c_{m} are calculated from the pure component parameters (a_i, b_i and c_i of component i) using the van der Waals mixing rule

$$a_{\mathrm{m}} = \sum_i \sum_j x_i x_j a_{ij} \tag{S10}$$

$$a_{ij} = (1 - k_{ij})\sqrt{a_i a_j} \tag{S11}$$

$$b_{\mathrm{m}} = \sum_i x_i b_i \tag{S12}$$

$$c_{\mathrm{m}} = \sum_i x_i c_i \tag{S13}$$

where x_i is the mole fraction of component i, and k_{ij} is the binary interaction parameter, which could be considered constant for each binary mixture.

For mixtures, defining terms:

$$d_{\mathrm{m}} = \left[b_{\mathrm{m}} c_{\mathrm{m}} + \frac{(b_{\mathrm{m}} + c_{\mathrm{m}})^2}{4} \right]^{1/2}, q_{\mathrm{m}} = \frac{b_{\mathrm{m}} + c_{\mathrm{m}}}{2} + d_{\mathrm{m}}, m_{\mathrm{m}} = \frac{b_{\mathrm{m}} + c_{\mathrm{m}}}{2} - d_{\mathrm{m}} \tag{S14}$$

The molar residual entropy s^{r}, molar residual enthalpy h^{r}, and molar residual isobaric heat capacity cr p can be calculated with:

$$s^{\mathrm{r}} = R \ln \frac{v - b_{\mathrm{m}}}{v} - \frac{1}{2d_{\mathrm{m}}} \frac{\mathrm{d}a_{\mathrm{m}}}{\mathrm{d}T} \ln \frac{v + m_{\mathrm{m}}}{v + q_{\mathrm{m}}} \tag{S15}$$

$$h^{\mathrm{r}} = \frac{RTb_{\mathrm{m}}}{v - b_{\mathrm{m}}} - \frac{a_{\mathrm{m}}}{2d_{\mathrm{m}}} \left(\frac{1}{v + m_{\mathrm{m}}} - \frac{1}{v + q_{\mathrm{m}}} \right) + \frac{1}{2d_{\mathrm{m}}} \left(a_{\mathrm{m}} - T \frac{\mathrm{d}a_{\mathrm{m}}}{\mathrm{d}T} \right) \ln \frac{v + m_{\mathrm{m}}}{v + q_{\mathrm{m}}} \tag{S16}$$

$$c_p^{\mathrm{r}} = -\frac{T}{2d_{\mathrm{m}}} \frac{\mathrm{d}^2 a_{\mathrm{m}}}{\mathrm{d}^2 T} \ln \frac{v + m_{\mathrm{m}}}{v + q_{\mathrm{m}}} - R - T \left(\frac{\partial p}{\partial T} \right)_v^2 \Big/ \left(\frac{\partial p}{\partial v} \right)_T \tag{S17}$$

Here, the derivatives $\mathrm{d}a_{\mathrm{m}}/\mathrm{d}T$ and $\mathrm{d}^2 a_{\mathrm{m}}/\mathrm{d}^2 T$ are calculated according to Eq. (S7), and the partial derivatives in Eq. (S17) are calculated according to Eq. (S6). Eqs. (S14) to (S17) without subscript 'm' are used for pure and quasi-pure fluids.

Table S1: Summary of the studied cubic equations of state.

EoS [a]	Ω_a	Ω_b	Ω_c	α
PR	0.45724	0.07779	0.07779	$\alpha = (1+m\cdot(1-T_r^{1/2}))^2$ $m = 0.37464+1.54226\omega-0.26992\omega^2$ $(\omega\leq 0.49)$ $m = 0.37964+1.48503\omega-0.164423\omega^2+0.016666\omega^3$ $(\omega>0.49)$;
RK	0.42748	0.08664	0	$\alpha = T_{r,i}^{-1/2}$;
PTV	$0.66121 - 0.761057\cdot Z_C$	$0.02207 + 0.20868\cdot Z_C$	$0.57765 - 1.87080\cdot Z_C$	$\alpha = (1+m\cdot(1-T_r^{1/2}))^2$; Z_C is compression factor at critical point. $m = 0.46283 + 3.58230\omega Z_C + 8.19417(\omega Z_C)^2$;
PRSV	0.45724	0.07779	0.07779	$\alpha = (1+m\cdot(1-T_r^{1/2}))^2$ $m = m_0 + m_1\cdot(1+T_r^{1/2})\cdot(0.7-T_r)$ $m_0 = 0.378893+1.4897153\omega-0.17131848\omega^2+0.0196554\omega^3$ $m_1 = 0$ ($T_r > 0.7$); otherwise value in Table 1 of Ref. [44]
SRK	0.42748	0.08664	0	$\alpha = (1+m\cdot(1-T_r^{1/2}))^2$ $m = 0.48508 +1.55171\omega-0.15613\omega^2$;
WRK	0.42748	0.08664	0	$\alpha = T_r\cdot(1+m\cdot(T_r^{-1}-1))$ $m = 1.57 +1.62\omega$

[a] Peng-Robinson (PR) [5], Redlich-Kwong (RK) [6], Patel-Teja-Valderrama (PTV) [3,4], Peng-Robinson-Stryjek-Vera (PRSV) [7], Soave-Redlich-Kwong (SRK) [8,9] and Wilson-Redlich-Kwong (WRK) [10] Equation of state (EoS).

S1.4 Ideal gas heat capacity

For pure fluids, a correlation of the ideal-gas isobaric heat capacity co p as a linear function of temperature is adopted:

$$c_{\mathrm{p}}^{\mathrm{o}} = k_1 \frac{(T - T_0)}{T_{\mathrm{c}}} + k_0 \tag{S18}$$

where k_0 is the value of co p at temperature T_0 = 298.15 K, and k_1/T_{c} is the gradient of co p at T_0. The ideal gas enthalpy h^{o} and entropy s^{o} and Helmholtz energy l^{o} can be calculated with:

$$k_2 = k_0 - \frac{k_1 T_0}{T_{\mathrm{c}}} \tag{S19}$$

$$h^{\mathrm{o}} = \int_{T_{\mathrm{ref}}}^{T} c_p^{\mathrm{o}} dT = \frac{k_1}{2T_{\mathrm{c}}}\left(T^2 - T_{\mathrm{ref}}^2\right) + k_2(T - T_{\mathrm{ref}}) \tag{S20}$$

$$s^{\mathrm{o}} = R\ln\frac{v}{v_{\mathrm{ref}}} + \frac{k_1}{T_{\mathrm{c}}}(T - T_{\mathrm{ref}}) + (k_2 - R)\ln\frac{T}{T_{\mathrm{ref}}} \tag{S21}$$

$$l^{\mathrm{o}} = h^{\mathrm{o}} - R \cdot T - s^{\mathrm{o}} \cdot T \tag{S22}$$

The values of (T_{ref}, v_{ref}) are the reference state for enthalpy and entropy, and can be selected arbitrarily. For mixtures,

$$l_{\mathrm{mix}}^{\mathrm{o}} = \sum_i x_i \cdot (l^{\mathrm{o}} + R \cdot T \cdot \ln(x_i)) \tag{S23}$$

$$s_{\mathrm{mix}}^{\mathrm{o}} = -\sum_i x_i \cdot \left(\frac{dl_i^{\mathrm{o}}}{dT} + R \cdot \ln(x_i)\right) \tag{S24}$$

$$h_{\mathrm{mix}}^{\mathrm{o}} = l_{\mathrm{mix}}^{\mathrm{o}} + R \cdot T + s_{\mathrm{mix}}^{\mathrm{o}} \cdot T \tag{S25}$$

$$c_{\mathrm{p,mix}}^{\mathrm{o}} = \sum_i x_i \cdot c_{\mathrm{p},i}^{\mathrm{o}} \tag{S26}$$

S1.5 Viscosity model

The viscosity of pure fluids is calculated as the sum of the dilute gas viscosity $\mu_{\rho\to 0}$ and the residual part μ^{r}:

$$\mu = \mu_{\rho\to 0} + \mu^{\mathrm{r}} \tag{S27}$$

The dilute gas viscosity $\mu_{\rho\to 0}$ of a pure fluid is calculated with the Chapman-Enskog [11] solution of the Boltzmann transport equation, assuming the interactions between molecules can be roughly captured by those of Lennard-Jones (L-J) particles:

$$\mu_{\rho\to 0} = \frac{5}{16}\sqrt{\frac{mk_BT}{\pi}}\frac{1}{\sigma^2\Omega^{(2,2)*}} \tag{S28}$$

where m, in units of kg, is the mass of one molecule, k_B, with the value of $1.380649\cdot10^{-23}$ J·K^{-1}, is the Boltzmann constant, σ is the collision diameter of a L-J 12-6 particle, and $\Omega^{(2,2)*}$ is the reduced collision integral obtained by integrating the possible approach trajectories of the particles. Neufeld et al.[12] gave an empirical correlation of $\Omega^{(2,2)*}$ as a function of temperature as:

$$\Omega^{(2,2)*} = 1.16145\cdot T^{*\,-0.14874} + 0.52487\cdot e^{-0.77320\cdot T^*} + 2.16178\cdot e^{-2.43787\cdot T^*} \tag{S29}$$

where $T^* = k_BT/\varepsilon$ is the dimensionless temperature, and ε/k_B is the reduced L-J pair-potential energy.

According to the residual entropy approach of Yang et al. [13], the residual part of viscosity μ^r can be calculated with:

$$\mu^r = \frac{\mu^r + \rho_N^{2/3}\sqrt{mk_BT}}{(s^+)^{2/3}} \tag{S30}$$

$$\ln(\mu^{r+} + 1) = n_{\mu1}\cdot(s^+) + n_{\mu2}\cdot(s^+)^{1.5} + n_{\mu3}\cdot(s^+)^2 + n_{\mu4}\cdot(s^+)^{2.5} \tag{S31}$$

$$s^+ = -s^r/R \tag{S32}$$

Here, ρ_N, in units of m^{-3}, is the number density. The number density ρ_N and residual entropy s^r are calculated with the methods provided in the Section S1.3. The four parameters $n_{\mu k}$ (k = 1,2,3,4) are fitted parameters for each pure or quasi-pure fluid.

For mixtures, the dilute gas viscosity $\eta_{\rho\to0,\mathrm{mix}}$ is calculated with the approximation of Wilke [14]:

$$\eta_{\rho\to0,\mathrm{mix}} = \sum_{i=1}^{N}\frac{x_i\cdot\eta_{\rho\to0,i}}{\sum_{j=1}^{N}x_j\cdot\varphi_{ij}} \tag{S33}$$

$$\varphi_{ij} = \frac{\left(1+(\eta_{\rho\to0,i}/\eta_{\rho\to0,j})^{1/2}\cdot(m_j/m_i)^{1/4}\right)^2}{(8\cdot(1+m_i/m_j))^{1/2}}, \tag{S34}$$

where m_i is the mass of one molecule of component i. In Eq. (S30), the mole fraction weighted average m_{mix} of the components is used to replace the effective mass of one particle m:

$$m_{\mathrm{mix}} = \sum_i x_i \cdot m_i \tag{S35}$$

In Eq. (S31), the mole fraction weighted average coefficient $n_{\mu k,\mathrm{mix}}$ is utilised to substitute the parameters $n_{\mu k,i}$, i.e.,

$$n_{\mu k,\mathrm{mix}} = \sum_i x_i \cdot n_{\mu k,i} \tag{S36}$$

where $n_{\mu k,i}$ (k = 1,2,3,4) are fitted $n_{\mu k}$ parameters of component i. The number density ρ_{N} and residual entropy s^{r} are calculated with the methods provided in the Section S1.3 for mixtures.

S1.6 Thermal conductivity model

The fluid thermal conductivity is calculated as the sum of the dilute gas term $\lambda_{\rho\to 0}$, the residual part λ^{r} and the critical enhancement of thermal conductivity $\Delta\lambda_{\mathrm{C}}$:

$$\lambda = \lambda_{\rho\to 0} + \lambda^{\mathrm{r}} + \lambda_{\mathrm{C}} \tag{S37}$$

The dilute gas thermal conductivity $\lambda_{\rho\to 0}$ is calculated according to the method in Chichester and Huber [15].

$$\lambda_{\rho\to 0} = \frac{f_{\mathrm{int}} \cdot \mu_{\rho\to 0}}{M}\left[c_p^0 - \frac{5}{2}R\right] + \frac{15 \cdot 10^{-3} R \cdot \mu_{\rho\to 0}}{4M} \tag{S38}$$

Here f_{int} is set to constant $1.32\cdot10^{-3}$ in this work although it could be a linear function of temperature in large temperature range.

According to the residual entropy approach of Yang et al. [16], the residual part of thermal conductivity λ^{r} can be calculated with:

$$\lambda^{\mathrm{r}+} = \frac{\lambda^{\mathrm{r}} + k_B \rho_{\mathrm{N}}^{2/3} \sqrt{k_B T/m}}{(s^+)^{2/3}} \tag{S39}$$

$$\lambda^{\mathrm{r}+} = n_{\lambda 1} \cdot (s^+) + n_{\lambda 2} \cdot (s^+)^{1.5} + n_{\lambda 3} \cdot (s^+)^2 + n_{\lambda 4} \cdot (s^+)^{2.5} \tag{S40}$$

The four parameters $n_{\lambda k}$ (k = 1,2,3,4) are fitted parameters for each pure fluid.

The critical enhancement of thermal conductivity $\Delta\lambda_{\mathrm{C}}$ is calculated according to a crossover model proposed by Olchowy and Sengers [17] as

$$\Delta\lambda_{\mathrm{C}} = \frac{\rho c_p R_{\mathrm{D}} k_{\mathrm{B}} T}{6\pi\mu\varphi}(\overline{\Omega} - \overline{\Omega}_0) \tag{S41}$$

$$\overline{\Omega} = \frac{2}{\pi}\left[\left(\frac{c_p - c_v}{c_p}\right)\arctan\left(q_{\mathrm{D}}\varphi\right) + \frac{c_v}{c_p}q_{\mathrm{D}}\varphi\right] \tag{S42}$$

$$\overline{\Omega}_0 = \frac{2}{\pi}\left[1 - \exp\left(-\frac{1}{(q_{\mathrm{D}}\varphi)^{-1} + (q_{\mathrm{D}}\varphi\rho_{\mathrm{c}}/\rho)^2/3}\right)\right] \tag{S43}$$

$$\varphi = \varphi_0\left(\frac{p_{\mathrm{c}}\rho}{\Gamma{\rho_{\mathrm{c}}}^2}\right)^{\nu/\gamma}\left[\left.\frac{\partial\rho(T,p)}{\partial p}\right|_T - \left(\frac{T_{\mathrm{ref}}}{T}\right)\left.\frac{\partial\rho(T_{\mathrm{ref}},p)}{\partial p}\right|_T\right]^{\nu/\gamma} \tag{S44}$$

Here c_v and c_p are the isobaric and isochoric specific heat capacity, the values of $R_{\mathrm{D}} = 1.02$, $\nu = 0.63$, and $\gamma = 1.239$ are universal constants, T_{ref} is generally $1.5\cdot T_{\mathrm{C}}$, while Γ, φ_0, and q_{D} are fluid-specific parameters.

For mixtures, the dilute gas thermal conductivity $\lambda_{\rho\to0,\mathrm{mix}}$ is calculated using Eqs. (S33) and (S34) but with η replaced by λ. Similarly, $n_{\lambda k,\mathrm{mix}}$ (k = 1,2,3,4) are calculated using Eq. (S36) with η replaced by λ. What different with viscosity calculation is that, in Eq. (S39), the mass fraction (instead of mole fraction) weighted average m_{mix} of the components is used to replace the effective mass of one particle m:

$$m_{\mathrm{mix}} = \sum_i y_i \cdot m_i \tag{S45}$$

where y_i is the mass fraction of component i. At last, the three parameters Γ, φ_0 and q_{D}, and the critical parameters (T_{crit}, ρ_{crit} and p_{crit}) of the mixtures needed for critical enhancement of the thermal conductivity calculation in Eqs. (S41) to (S44) are roughly replaced with the mole-fraction-weighted average of the pure components.

S2. Tables in the feasibility study

See the following pages.

Table S2. Reference values of the constants of real fluids. [a]

Fluid	M	T_c /K	p_c MPa	ω	k_0 /J·mol^{-1}·K^{-1}	k_1 /J·mol^{-1}·K^{-1}	ε/k_B /K	σ /nm	$\varphi_0 \cdot 10^{10}$	Γ	$q_D^{-1} \cdot 10^{10}$
C11	156.308	638.800	1.9904	0.5390	255.753	398.630	445.750	0.7815	2.67	0.059	8.660
C12	170.335	658.100	1.8170	0.5740	278.301	440.856	522.592	0.7356	1.94	0.050	15.200
C1CC6	98.186	572.200	3.4700	0.2340	136.137	256.835	281.100	0.5943	1.50	0.052	6.240
C3CC6	126.239	630.800	2.8600	0.3260	184.502	347.895	500.910	0.6358	1.50	0.052	6.240
CHLOROBENZENE	112.557	632.350	4.5206	0.2532	98.022	154.886	502.100	0.5470	1.60	0.098	6.660
D5	370.770	618.300	1.0934	0.6370	510.297	412.520	491.000	0.8640	3.19	0.064	10.680
D6	444.924	645.780	0.9610	0.7360	566.136	612.730	512.800	0.9450	3.41	0.072	11.700
DECANE	142.282	617.700	2.1030	0.4884	233.025	356.560	490.510	0.6860	1.94	0.050	7.086
EBENZENE	106.165	617.120	3.6224	0.3050	127.526	225.408	490.050	0.5781	2.35	0.056	7.060
HEPTANE	100.202	540.200	2.7357	0.3490	165.238	228.932	400.000	0.6495	2.45	0.059	8.000
IOCTANE	114.229	544.000	2.5720	0.3030	184.807	288.317	431.990	0.6300	2.56	0.059	7.710
MD2M	310.685	599.400	1.1440	0.6350	416.848	440.909	476.000	0.8490	3.11	0.066	10.490
MD3M	384.839	628.960	0.9611	0.7230	523.443	566.140	499.500	0.9110	3.30	0.066	11.270
MD4M	458.993	653.200	0.8404	0.8060	619.538	682.143	518.700	0.9760	3.47	0.070	12.080
MDM	236.532	565.361	1.4375	0.5240	329.268	348.229	447.940	0.7704	2.95	0.064	9.560
MILPRF23699	557.600	930.000	1.0800	0.9700	737.539	1315.890	738.506	1.0644	3.65	0.087	13.200
MLINOLEA	294.472	799.000	1.3410	0.8050	432.040	699.456	634.500	0.8700	1.94	0.050	8.750
MLINOLEN	292.456	772.000	1.3690	1.1400	418.995	667.050	613.040	0.8549	2.84	0.073	10.560
MM	162.377	518.700	1.9311	0.4180	238.357	229.935	357.000	0.7190	2.68	0.062	8.400
MOLEATE	296.488	782.000	1.2460	0.9060	445.205	710.531	621.000	0.8700	1.94	0.050	8.750
MXYLENE	106.165	616.890	3.5346	0.3260	125.574	217.710	489.870	0.5800	2.35	0.057	7.130
NONANE	128.255	594.550	2.2810	0.4433	210.411	314.397	472.127	0.6638	1.94	0.050	10.431
OCTANE	114.229	568.740	2.4836	0.3980	189.058	269.508	452.090	0.6362	1.94	0.050	6.863
OXYLENE	106.165	630.259	3.7375	0.3120	131.343	220.347	500.480	0.5820	2.36	0.058	7.110
POE5	472.612	890.000	1.2700	0.8900	597.857	1124.317	706.742	0.9838	3.43	0.082	12.180
POE7	584.835	940.000	1.0300	1.0600	790.170	2055.401	746.446	1.0872	3.67	0.090	13.490
POE9	697.051	970.000	0.8850	0.9980	978.610	2899.618	770.269	1.1877	4.05	0.096	14.760
TOLUENE	92.138	591.750	4.1263	0.2657	103.791	186.961	469.900	0.5507	2.20	0.050	6.200
PROPANE	44.096	369.890	4.2512	0.1521	73.336	73.510	263.880	0.4975	1.94	0.050	7.166
CO_2	44.010	304.128	7.3773	0.2239	37.141	14.269	251.196	0.3751	1.50	0.052	4.000

[a] Values were obtained directly or fitted using data from REFPROP 10.0 [18].

Table S3. Values used for parameter fitting in the feasibility study. [a]

REFPROP fluid name	T / K	ρ / kg·m^{-3}	c_p / J·kg^{-1}·K^{-1}	μ / Pa·s	λ / W·m^{-1}·K^{-1}
C11	278.15	756.004	2185.93	0.001515	0.1395
C11	308.15	730.702	2249.76	0.000923	0.1312
C11	338.15	704.898	2394.92	0.000649	0.1265
C11	368.15	683.072	2533.02	0.000470	0.1152
C12	278.15	762.327	2183.90	0.002038	0.1434
C12	308.15	737.714	2310.49	0.001174	0.1334
C12	338.15	718.260	2357.39	0.000746	0.1275
C12	368.15	696.966	2517.85	0.000550	0.1200
C1CC6	278.15	781.703	1804.41	0.000920	0.1135
C1CC6	308.15	755.921	1924.67	0.000611	0.1067
C1CC6	338.15	729.662	2099.26	0.000434	0.0994
C1CC6	368.15	705.521	2254.92	0.000329	0.0913
C3CC6	278.15	809.844	1907.34	0.001303	0.1184
C3CC6	308.15	784.137	2040.57	0.000826	0.1101
C3CC6	338.15	758.182	2150.48	0.000570	0.1028
C3CC6	368.15	737.760	2240.65	0.000435	0.0980
CHLOROBENZENE	278.15	1127.504	1306.44	0.000967	0.1322
CHLOROBENZENE	308.15	1091.508	1384.80	0.000682	0.1220
CHLOROBENZENE	338.15	1063.901	1459.46	0.000498	0.1173
CHLOROBENZENE	368.15	1026.467	1501.93	0.000383	0.1113
D5	278.15	980.617	1738.68	0.006560	0.1247
D5	308.15	948.183	1730.58	0.003217	0.1155
D5	338.15	910.069	1798.01	0.001835	0.1078
D5	368.15	883.020	1828.82	0.001178	0.0981
D6	278.15	995.828	1548.74	0.010230	0.1261
D6	308.15	961.521	1598.66	0.005570	0.1161
D6	338.15	923.264	1652.02	0.003093	0.1105
D6	368.15	895.992	1693.48	0.001850	0.0988
DECANE	278.15	743.688	2171.06	0.001183	0.1348
DECANE	308.15	722.521	2276.24	0.000747	0.1302
DECANE	338.15	695.992	2356.42	0.000521	0.1186
DECANE	368.15	672.181	2465.56	0.000389	0.1142
EBENZENE	278.15	884.615	1723.03	0.000828	0.1316
EBENZENE	308.15	852.726	1796.91	0.000578	0.1282
EBENZENE	338.15	831.726	1934.34	0.000418	0.1182
EBENZENE	368.15	803.238	1984.49	0.000330	0.1138
HEPTANE	278.15	696.977	2212.70	0.000501	0.1311
HEPTANE	308.15	672.904	2271.20	0.000355	0.1182
HEPTANE	338.15	647.315	2448.42	0.000266	0.1102
HEPTANE	368.15	619.104	2590.79	0.000203	0.1010
IOCTANE	278.15	707.200	2024.97	0.000623	0.1021
IOCTANE	308.15	680.033	2193.46	0.000430	0.0922
IOCTANE	338.15	654.118	2337.43	0.000315	0.0845

IOCTANE	368.15	630.540	2468.86	0.000247	0.0781
MD2M	278.15	870.410	1699.46	0.001794	0.1190
MD2M	308.15	841.394	1766.77	0.001153	0.1087
MD2M	338.15	807.634	1865.50	0.000798	0.1011
MD2M	368.15	781.020	1921.08	0.000574	0.0922
MD3M	278.15	893.580	1670.92	0.002499	0.1176
MD3M	308.15	863.494	1781.12	0.001561	0.1117
MD3M	338.15	829.976	1804.92	0.001072	0.1070
MD3M	368.15	802.451	1856.73	0.000761	0.0991
MD4M	278.15	906.451	1666.56	0.003181	0.1331
MD4M	308.15	877.706	1729.69	0.002070	0.1261
MD4M	338.15	848.748	1826.60	0.001337	0.1177
MD4M	368.15	823.489	1894.40	0.000912	0.1118
MDM	278.15	834.343	1733.58	0.001087	0.1144
MDM	308.15	807.122	1807.84	0.000752	0.1051
MDM	338.15	774.670	1906.92	0.000522	0.0956
MDM	368.15	743.042	1989.41	0.000392	0.0884
MILPRF23699	278.15	1005.541	1742.07	0.144980	0.1523
MILPRF23699	308.15	985.650	1841.94	0.030498	0.1466
MILPRF23699	338.15	956.618	1917.57	0.010850	0.1410
MILPRF23699	368.15	939.282	2000.66	0.005249	0.1370
MLINOLEA	278.15	897.896	2385.41	0.007378	0.1459
MLINOLEA	308.15	874.340	2296.01	0.003585	0.1455
MLINOLEA	338.15	854.735	2353.64	0.002099	0.1391
MLINOLEA	368.15	836.935	2316.77	0.001384	0.1364
MLINOLEN	278.15	909.563	2150.00	0.006419	0.1480
MLINOLEN	308.15	890.840	2104.60	0.003335	0.1472
MLINOLEN	338.15	868.027	2157.65	0.001945	0.1401
MLINOLEN	368.15	848.153	2222.38	0.001321	0.1392
MM	278.15	784.843	1838.11	0.000597	0.1132
MM	308.15	750.571	1947.37	0.000441	0.1043
MM	338.15	716.482	2041.17	0.000332	0.0939
MM	368.15	684.616	2143.56	0.000236	0.0851
MOLEATE	278.15	888.028	2268.19	0.010403	0.1430
MOLEATE	308.15	862.085	2298.59	0.004494	0.1446
MOLEATE	338.15	846.273	2351.67	0.002404	0.1402
MOLEATE	368.15	824.182	2365.55	0.001564	0.1369
MXYLENE	278.15	875.670	1666.03	0.000749	0.1353
MXYLENE	308.15	853.350	1777.90	0.000524	0.1287
MXYLENE	338.15	824.124	1842.04	0.000389	0.1205
MXYLENE	368.15	797.591	1952.48	0.000310	0.1132
NONANE	278.15	731.979	2137.67	0.000863	0.1342
NONANE	308.15	707.284	2284.38	0.000590	0.1246
NONANE	338.15	683.998	2358.38	0.000433	0.1174
NONANE	368.15	657.846	2485.38	0.000331	0.1111
OCTANE	278.15	716.956	2204.19	0.000674	0.1323

OCTANE	308.15	693.924	2277.27	0.000455	0.1217
OCTANE	338.15	669.018	2424.99	0.000342	0.1133
OCTANE	368.15	641.451	2486.99	0.000263	0.1054
OXYLENE	278.15	896.504	1713.52	0.001035	0.1359
OXYLENE	308.15	868.006	1823.53	0.000669	0.1275
OXYLENE	338.15	841.817	1946.46	0.000484	0.1226
OXYLENE	368.15	815.992	1976.83	0.000365	0.1119
POE5	278.15	1030.707	1750.67	0.072451	0.1492
POE5	308.15	1006.355	1811.78	0.018019	0.1422
POE5	338.15	984.842	1873.42	0.007459	0.1389
POE5	368.15	955.662	1991.55	0.003849	0.1336
POE7	278.15	994.087	1799.15	0.096956	0.1547
POE7	308.15	967.941	1863.50	0.022688	0.1510
POE7	338.15	941.862	1954.62	0.008882	0.1484
POE7	368.15	925.419	2021.13	0.004684	0.1439
POE9	278.15	966.498	1876.22	0.154566	0.1606
POE9	308.15	943.975	1985.85	0.035039	0.1564
POE9	338.15	921.913	2020.33	0.013456	0.1488
POE9	368.15	899.381	2104.47	0.006795	0.1449
TOLUENE	278.15	885.870	1648.23	0.000738	0.1352
TOLUENE	308.15	856.380	1756.27	0.000499	0.1289
TOLUENE	338.15	824.236	1828.04	0.000368	0.1220
TOLUENE	368.15	797.665	1961.69	0.000288	0.1128

[a] Values are all calculated with REFPROP 10.0 [18] at atmosphere pressure (p = 0.1 MPa) and added with $(1+2t)\cdot U_{exp}/4$, where t is a random value between –1 to 1 and U_{exp} is the estimated expanded experimental uncertainty.

Table S4. Molar mass determination using the Raoult's law of boiling point elevation. [a]

REFPROP fluid name	$(T_{solution} - T_{solvent})$ / K	M_{ref} / g·mol^{-1}	M_{fit} / g·mol^{-1}	$(M_{fit} - M_{ref})/M_{ref}$
C11	0.2513	156.308	161.472	3%
C12	0.2298	170.335	176.534	4%
C1CC6	0.4194	98.186	96.724	-1%
C3CC6	0.3217	126.239	126.131	0%
CHLOROBENZENE	0.3682	112.557	110.194	-2%
D5	0.1111	370.770	365.184	-2%
D6	0.0919	444.924	441.596	-1%
DECANE	0.2904	142.282	139.721	-2%
EBENZENE	0.3706	106.165	109.484	3%
HEPTANE	0.4116	100.202	98.559	-2%
IOCTANE	0.3655	114.229	111.002	-3%
MD2M	0.1327	310.685	305.654	-2%
MD3M	0.1255	384.839	323.274	-16%
MD4M	0.1018	458.993	398.596	-13%
MDM	0.1694	236.532	239.528	1%
MILPRF23699	0.0613	557.600	661.761	19%

MLINOLEA	0.1544	294.472	262.695	-11%
MLINOLEN	0.1193	292.456	340.012	16%
MM	0.2434	162.377	166.711	3%
MOLEATE	0.1452	296.488	279.454	-6%
MXYLENE	0.3923	106.165	103.415	-3%
NONANE	0.3249	128.255	124.871	-3%
OCTANE	0.3529	114.229	114.956	1%
OXYLENE	0.3663	106.165	110.751	4%
POE5	0.1002	472.612	405.063	-14%
POE7	0.0937	584.835	432.996	-26%
POE9	0.0824	697.051	492.116	-29%
TOLUENE	0.4171	92.138	97.274	6%

[a] The boiling point elevation experiments are simulated as follows: 2.0 g of solute is added to 100.0 g of pure propane at 0.8 MPa, and the boiling temperature elevations from the solvent $T_{solvent}$ to the solution $T_{solution}$ are calculated using REFPROP 10.0 [18] with a bias $(1+2t)\cdot 0.01$ K added to imitate experimental uncertainty. Here t is a random value between –1 to 1. The reference molar mass M_{ref} is obtained from REFPROP 10.0.

S3. Tables for PAG68 and its mixture with propane

Table S5. Density measurements for the quasi-pure PAG68 and its mixture with propane. [a]

T / K	x_{PAG68}	ρ / kg·m^{-3}	T / K	x_{PAG68}	ρ / kg·m^{-3}
263.82	1	1014.88	263.35	0.7027	846.72
292.94	1	991.67	283.87	0.7027	827.56
323.66	1	967.61	262.77	0.4962	723.37
352.97	1	945.21	283.77	0.4962	699.85
383.22	1	922.56	303.40	0.4962	678.38
412.9	1	900.88	322.95	0.4962	654.63
264.14	0.9087	948.83	343.18	0.4962	628.72
283.93	0.9087	931.86	263.49	0.33	658.43
303.28	0.9087	915.52	273.22	0.33	648.07
323.88	0.9087	899.49	283.93	0.33	633.72
342.44	0.9087	884.56	293.32	0.33	621.79
363.3	0.9087	867.35	303.29	0.33	610.82
264.13	0.7937	886.55	322.96	0.33	583.9
283.82	0.7937	868.61	263.15	0	541.8
303.3	0.7937	850.97	283.15	0	514.73
323.821	0.7937	832.92	303.15	0	484.39
343.18	0.7937	816.68	323.15	0	448.87
363.3	0.7937	798.41	333.15	0	427.97
293.62	0.7027	816.33	343.15	0	403.62
312.81	0.7027	798.31	353.15	0	373.29
333.04	0.7027	779.25	358.15	0	353.96
353.08	0.7027	760.56			

[a] The pressure is 0.1 MPa. x_{PAG68} is mass fraction of PAG68.

Table S6. Heat capacity measurements for the quasi-pure PAG68.[a]

T / K	c_p / J·kg^{-1}·K^{-1}	T / K	c_p / J·kg^{-1}·K^{-1}	T / K	c_p / J·kg^{-1}·K^{-1}
236.23	1750	281.19	1860	326.15	1980
241.22	1760	286.19	1870	331.15	1990
246.22	1780	291.18	1890	336.14	2000
251.21	1790	296.18	1900	341.14	2010
256.21	1800	301.17	1910	346.13	2030
261.21	1820	306.17	1930	351.13	2040
266.2	1830	311.16	1940	356.13	2050
271.2	1840	316.16	1950	356.13	2060
276.19	1850	321.16	1960		

[a] The pressures is 0.1 MPa.

Table S7. Thermal conductivity measurements for the quasi-pure PAG68 and the mixtures of PAG68 and propane.[a]

T / K	y_{PAG68}	λ / W·m^{-1}·K^{-1}	T / K	x_{PAG68}	λ / W·m^{-1}·K^{-1}
253.33	1	0.15231	273.31	0.1871	0.11113
273.32	1	0.14833	253.31	0.1871	0.12300
293.33	1	0.14694	293.32	0.1871	0.10023
253.32	1	0.15332	293.30	0.4952	0.11953
273.31	1	0.14812	273.29	0.4952	0.12835
293.32	1	0.14482	253.29	0.4952	0.13525

[a] The pressures is 0.3 MPa. y_{PAG68} is mass fraction of PAG68.

Table S8. Bubble-point pressure measurements for the mixtures of PAG68 and propane.[a]

T / K	w_{PAG68}	p_{bub} / MPa	T / K	w_{PAG68}	p_{bub} / MPa
232.58	0.8998	0.07599	363.23	0.8185	2.82684
241.89	0.9000	0.10864	241.39	0.7080	0.15437
253.23	0.9004	0.16191	253.14	0.7084	0.23686
263.17	0.9007	0.22253	263.16	0.7087	0.33117
273.16	0.9011	0.29835	273.16	0.7091	0.45106
283.17	0.9016	0.39127	283.14	0.7096	0.60042
293.17	0.9021	0.50219	293.11	0.7101	0.78317
303.22	0.9027	0.63331	303.23	0.7107	1.00419
313.71	0.9033	0.79201	313.33	0.7113	1.27169
323.69	0.9039	0.96454	323.32	0.7121	1.58497
333.70	0.9045	1.15826	333.19	0.7128	1.94654
343.70	0.9052	1.37418	343.22	0.7137	2.36708
353.70	0.9058	1.61050	353.28	0.7146	2.85119
363.70	0.9063	1.86692	233.78	0.9438	0.05445
232.11	0.8068	0.09881	243.39	0.9440	0.07768
241.31	0.8071	0.14236	253.23	0.9441	0.10901

253.15	0.8075	0.21641	263.16	0.9443	0.14893
263.16	0.8080	0.30093	273.17	0.9446	0.19835
273.14	0.8086	0.40705	283.17	0.9448	0.25767
283.14	0.8092	0.53887	293.11	0.9451	0.32720
293.09	0.8100	0.69850	303.21	0.9454	0.40871
303.20	0.8109	0.89201	313.70	0.9457	0.50502
313.31	0.8119	1.12053	323.20	0.9460	0.60265
323.29	0.8130	1.38305	333.21	0.9463	0.71558
333.20	0.8142	1.68098	343.21	0.9466	0.83890
343.30	0.8155	2.02509	353.44	0.9469	0.97531
353.44	0.8170	2.41171	363.66	0.9472	1.12012

[a] w_{PAG68} is mass fraction of PAG68.

Table S9. Viscosity measurements for the quasi-pure PAG68 and its mixture with propane.[a]

T / K	w_{PAG68}	μ / mPa·s	T / K	w_{PAG68}	μ / mPa·s
323.34	1	45.72	324.39	0.7027	2.11
323.25	1	45.16	323.43	0.7027	2.24
333.22	1	32.64	323.5	0.7027	2.26
333.18	1	32.37	334.03	0.7027	1.78
343.16	1	24.01	334	0.7027	1.79
343.1	1	23.89	333.02	0.7027	1.95
353.11	1	18.25	332.97	0.7027	1.91
362.97	1	14.51	344	0.7027	1.53
363.01	1	14.57	343.97	0.7027	1.54
303.23	1	101.58	342.81	0.7027	1.69
314.21	1	63.13	342.81	0.7027	1.67
313.13	1	64.43	353.91	0.7027	1.35
324.2	1	43.24	354	0.7027	1.32
323.03	1	42.94	363.63	0.7027	1.16
278.84	0.9087	53.43	363.84	0.7027	1.19
278.79	0.9087	51.52	238.27	0.7027	28.61
283.73	0.9087	42.52	243.84	0.7027	22.15
283.68	0.9087	39.58	243.79	0.7027	21.21
293.59	0.9087	28.24	253.28	0.7027	13.83
293.55	0.9087	26.51	253.44	0.7027	14.31
303.41	0.9087	19.31	263.67	0.7027	9.37
303.49	0.9087	19.65	263.77	0.7027	9.72
313.39	0.9087	14.57	273.49	0.7027	7.12
313.33	0.9087	14.07	273.45	0.7027	6.88
323.4	0.9087	11.36	273.97	0.7027	6.94
323.4	0.9087	10.77	273.94	0.7027	6.54
333.19	0.9087	8.94	285.24	0.7027	4.96
333.15	0.9087	8.83	285.21	0.7027	4.72
353.08	0.9087	6.4	284.67	0.7027	5.2

353.01	0.9087	6.31	284.62	0.7027	5.06
364.1	0.9087	4.81	238.37	0.4962	2.73
364.05	0.9087	5	238.13	0.4962	2.58
362.95	0.9087	5.11	242.75	0.4962	2.34
362.9	0.9087	5.09	242.72	0.4962	2.27
247.83	0.7937	44.31	252.44	0.4962	1.79
247.76	0.7937	42.44	252.38	0.4962	1.75
252.47	0.7937	32.65	263.74	0.4962	1.34
252.57	0.7937	34.29	263.06	0.4962	1.37
263.16	0.7937	20.67	263.66	0.4962	1.33
263.13	0.7937	19.51	263.04	0.4962	1.36
273.91	0.7937	13.41	273.57	0.4962	1.1
273.86	0.7937	13.04	273.44	0.4962	1.1
283.71	0.7937	9.38	272.73	0.4962	1.12
283.8	0.7937	9.72	272.73	0.4962	1.12
293.67	0.7937	7.32	283.3	0.4962	0.92
293.6	0.7937	7.12	283.43	0.4962	0.91
294.29	0.7937	7.15	282.47	0.4962	0.93
294.23	0.7937	7	282.55	0.4962	0.91
303.44	0.7937	5.61	294.22	0.4962	0.75
303.48	0.7937	5.69	294.37	0.4962	0.76
304.13	0.7937	5.64	293.33	0.4962	0.77
304.18	0.7937	5.74	293.41	0.4962	0.74
314.15	0.7937	4.46	303.18	0.4962	0.66
314.1	0.7937	4.42	303.33	0.4962	0.66
313.36	0.7937	4.6	302.19	0.4962	0.67
313.34	0.7937	4.53	302.29	0.4962	0.64
324.1	0.7937	3.56	313.16	0.4962	0.56
324.07	0.7937	3.45	313.31	0.4962	0.57
323.26	0.7937	3.75	312.12	0.4962	0.56
323.21	0.7937	3.69	312.19	0.4962	0.51
334.07	0.7937	2.91	323.63	0.4962	0.49
334.03	0.7937	2.9	323.8	0.4962	0.5
333.11	0.7937	3.15	322.47	0.4962	0.48
333.08	0.7937	3.1	322.58	0.4962	0.42
344.03	0.7937	2.68	333.67	0.4962	0.44
344.08	0.7937	2.61	333.53	0.4962	0.43
342.96	0.7937	2.66	343.7	0.4962	0.39
343.03	0.7937	2.67	343.5	0.4962	0.38
354.09	0.7937	2.18	238.48	0.33	0.81
354.05	0.7937	2.29	238.48	0.33	0.83
352.91	0.7937	2.36	242.69	0.33	0.72
352.85	0.7937	2.31	242.6	0.33	0.75
364.14	0.7937	1.85	252.34	0.33	0.57
364.01	0.7937	1.9	252.28	0.33	0.65
362.72	0.7937	1.96	262.84	0.33	0.47

362.66	0.7937	1.99	262.83	0.33	0.51
362.66	0.7937	1.99	272.68	0.33	0.36
294.81	0.7027	3.82	272.69	0.33	0.42
294.75	0.7027	3.67	282.56	0.33	0.3
294.2	0.7027	4.07	282.5	0.33	0.36
294.14	0.7027	3.97	293.33	0.33	0.32
304.63	0.7027	3.06	303.32	0.33	0.32
304.6	0.7027	3.01	303.19	0.33	0.31
303.94	0.7027	3.08	313.29	0.33	0.28
303.89	0.7027	3.22	313.15	0.33	0.27
314.33	0.7027	2.52	323.32	0.33	0.25
314.27	0.7027	2.47	323.15	0.33	0.24
313.55	0.7027	2.7	333.29	0.33	0.22
313.46	0.7027	2.65	333.13	0.33	0.21
324.33	0.7027	2.09		0	0

[a] The pressure is 0.1 MPa. w_{PAG68} is mass fraction of PAG68.

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