Supporting Information

Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment

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This supplementary material of the publication *Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment* contains the following:

1. The full database of thermophysical property data of the Lennard-Jones fluid discussed in this work is appended as an `.xls`-spreadsheet, including an indication for each bulk data point whether it was identified as an outlier by the EOS test.

2. Applied conversions for each property in a given publication included in the database to indicate how the values in the database were obtained from those printed in the publication. Also, remarks on individual publications are given regarding possible misprints, conversion pitfalls, outliers etc.

3. Additional information on the EOS test for the assessment of the homogeneous state points.

4. Details on the computation of thermophysical properties with the *Lustig* formalism.

5. Additional information on the compressibility factor test, the Clausius-Clapeyron test, and the deviation test of the VLE bulk data, cf. Fig. S2, S3, and S4, respectively. All available VLE data (both confirmed and discarded) are shown and discussed in detail.

6. Additional information on the surface tension data, cf. Fig. S5.

7. List of clear outliers (eight data point) from the seven best VLE data sets (Refs.[23,71,121,122,125–127,135,136] and this work), cf. Table S4.

8. Numerical values of the VLE data set from this work, cf. Table S3.

Database: `.xls`-spreadsheet

The entire database of thermophysical properties considered in this work is provided as an *.xls* spreadsheet in the electronic supplementary material.

List of applied conversions and remarks

For all considered studies in the database, the applied conversions from the numerical values printed in a publication to obtain the numerical values given in the database are given in Table S1. Data are consistently reported as residual properties (with respect to the ideal gas) and in the standard 'Lennard-Jones' units.

In Table S1, the hat $\hat{}$ indicates the obtained value after the conversion as given in the database. Non-hat symbols were adopted as it stands in the corresponding publication. The asterisk indicates 'Lennard-Jones' units. Non-asterisk values indicate other units systems as applied in a given publication. The tilde $\tilde{a}$ indicates the Helmholtz energy per particle a divided by the temperature, i.e. $\tilde{a} = \frac{a}{T}$. The [Acronym] indicates the string used in the electronic database to uniquely identify a certain publication. The *state point* is the given temperature and density and their respective conversions in case of homogeneous data; and only the temperature in case of VLE data. The column *property* lists the given thermophysical properties and their respective conversions of a given publication.

In cases where multiple results where reported for a given property and state point in a given publication (e.g. simulations performed with varying cut-off, particle number, sampling length etc.), only the numeric value with the largest particle number etc. were included in the database.

For the conversions given in Table S1, the constants $N_{\mathrm{AV}} = 6.02214076 \cdot 10^{23}\,\mathrm{mol}^{-1}$ and $k_{\mathrm{B}} = 1.380649 \cdot 10^{-23}\,\mathrm{J} \cdot \mathrm{K}^{-1}$ were applied.

For the studies that report data based on the *Lustig* formalism, the Helmholtz energy and the respective derivatives are listed in Table S1. According the thermodynamic relations (see below), other properties were computed from that data and also included in the database.

Table S1: List of conversions from the publications from the literature to the consistent units system (Lennard-Jones units & residual properties with respect to the ideal gas).

Authors & **[Acronym]**	**state point** T, ρ	**thermophysical** **properties**
Wood and Parker[15]	$\widehat{T}^* = T^*$	$\widehat{c}_v^* = \frac{3}{2} + C_v'/R$
[WOODPAR]	$\widehat{\rho}^* = \left(\frac{v}{v^*}\right)^{-1}$	$\widehat{u}_{\mathrm{res}}^* = \widehat{T}^* \cdot \frac{E'}{RT}$
		$\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot \frac{pv}{RT}$
Hansen[50]	$\widehat{T}^* = T^*$	$\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot (\frac{\beta p}{\rho})^{\mathrm{ex}}$
[HANSEN]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}_{\mathrm{res}}^* = \widehat{T}^* \cdot (\beta U)^{\mathrm{ex}}$
Levesque and Verlet[48]	$\widehat{T}^* = T^*$	$\widehat{a}_{\mathrm{res},00}^* = \frac{F_1}{N \cdot k_{\mathrm{B}} \cdot T}$
[LEVEVER]	$\widehat{\rho}^* = \rho^*$	$\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot Z$
		$\widehat{u}_{\mathrm{res}}^* = u_i$
Thol et al.[90]	$\widehat{T}^* = T^*$	$\widehat{a}_{\mathrm{res},00}^* = A_{\mathrm{r},00}$
[THOL]	$\widehat{\rho}^* = \rho^*$	$\widehat{a}_{\mathrm{res},01}^* = A_{\mathrm{r},01}$
		$\widehat{a}_{\mathrm{res},10}^* = A_{\mathrm{r},10}$
		$\widehat{a}_{\mathrm{res},11}^* = A_{\mathrm{r},11}$
		$\widehat{a}_{\mathrm{res},02}^* = A_{\mathrm{r},02}$
		$\widehat{a}_{\mathrm{res},20}^* = A_{\mathrm{r},20}$
The numeric values provided in the supplementary material in Ref.[90] contains some typos. Those are corrected here.		
Verlet[18]	$\widehat{T}^* = T^*$	$\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot (\frac{\beta p}{\rho})$
[VERLET]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}_{\mathrm{res}}^* = U^i$
Hansen and Verlet[20]	$\widehat{T}^* = T^*$	$\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot \frac{\beta p}{\rho}$
[HANSVER]	$\widehat{\rho}^* = \rho^*$	$\widehat{a}_{\mathrm{res},00}^* = \frac{F_l}{\widehat{T}^*} - \ln(\widehat{\rho}^*) + 1$
		$\widehat{p}_v^* = p_v^*$
		$\Delta\widehat{h_v}^* = \mathcal{L}$
McDonald and Singer[54]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$

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Authors & [Acronym]	state point T, ρ	thermophysical properties
[MCDSING]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_r$
Weeks et al.[160]	$\widehat{T}^* = T^*$	$\widehat{\widehat{a}}^*_{\mathrm{res},00} = -\frac{\beta \Delta A}{N}$
[WEEKCHA1]	$\widehat{\rho}^* = \rho^*$	
Adams[57]	$\widehat{T}^* = T^*$	$\widehat{\alpha}^* = \alpha^*$
[ADAMS]	$\widehat{\rho}^* = \rho^*$	$\widehat{\beta}^* = \beta^*$
		$\widehat{\gamma}^* = \gamma^*$
		$\widehat{p}^* = p*$
		$\widehat{\mu}^*_{\mathrm{res}} = \mu^*_r$
		$\widehat{u}^*_{\mathrm{res}} = -u^*_r$
		$\widehat{c}^*_v = \frac{3}{2} + c^*_{v,r}$
Ree[62]	$\widehat{T}^* = T^*$	$\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot \frac{P}{\rho k T}$
[REE]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = \frac{U^e}{kT} \cdot \widehat{T}^*$
Panagiotopoulos[100]	$\widehat{T}^* = T^*$	$\widehat{p}^*_v = P^*$
[PANAGIO]	$\widehat{\rho}^* = \rho^*$	$\Delta \widehat{h}^*_v = (E^*_{\mathrm{v}} + \frac{\widehat{p}^*_{\mathrm{v}}}{\widehat{\rho}^*_{\mathrm{v}}} - (E^*_{\mathrm{l}} + \frac{\widehat{p}^*_{\mathrm{l}}}{\widehat{\rho}^*_{\mathrm{l}}}))$
Shaw[66]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[SHAW]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_r$
Panagiotopoulos et al.[101]	$\widehat{T}^* = T^*$	$\widehat{p}^*_v = P$
[PANQUIR]	$\widehat{\rho}^* = \rho^*$	$\Delta \widehat{h}^*_v = (E^{\mathrm{G}} + \frac{p^{\mathrm{G}}}{\rho^{\mathrm{G}}} - (E^{\mathrm{L}} + \frac{p^{\mathrm{L}}}{\rho^{\mathrm{L}}}))$
Smit and Frenkel[103]	$\widehat{T}^* = T^*$	$\Delta \widehat{h}^*_v = (E^*_{\mathrm{v}} + \frac{\widehat{P}^*_{\mathrm{v}}}{\widehat{\rho}^*_{\mathrm{v}}} - (E^*_{\mathrm{l}} + \frac{\widehat{p}^*_{\mathrm{l}}}{\widehat{\rho}^*_{\mathrm{l}}}))$
[SMITFRE]	$\widehat{\rho}^* = \rho^*$	$\widehat{p}^*_v = p^*_v$
Meier[80,155]	$\widehat{T}^* = T^*$	$\widehat{c}^*_v = c^*_v$
[MEIER]	$\widehat{\rho}^* = \rho^*$	$\widehat{p}^* = p^*$
		$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
		$\widehat{w}^* = w'^*_o$
		$\widehat{\gamma}^* = \gamma^*$

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Authors & [Acronym]	**state point** T, ρ	**thermophysical properties**
Two typos in Ref.[80] are known[155] that were corrected in the database: A '0' is missing for the numbers of the reported pressure of two state points ($\widehat{\rho}^* = 0.01$ & $\widehat{T}^* = 0.900501$ and $\widehat{\rho}^* = 0.005$ & $\widehat{T}^* = 0.900929$).		
Johnson et al.[73]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[JOHNSON]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_r$
Hunter and Reinhardt[107]	$\widehat{T}^* = T^*$	$\widehat{p}^*_v = p^*_v$
[HUNTERR]	$\widehat{\rho}^* = \rho^*$	
McDonald and Singer[45]	$\widehat{T}^* = \frac{T \cdot k_{\mathrm{B}}}{\varepsilon}$	$\widehat{p}^* = \frac{10^{-23} \cdot \sigma^3 \cdot p^*}{\varepsilon}$
[MCDSIN1]	$\widehat{\rho}^* = \frac{10^{-24} \cdot \sigma^3 \cdot N_{\mathrm{AV}}}{v}$	$\widehat{u}^*_{\mathrm{res}} = -u^*_{\mathrm{r}} \cdot \widehat{T}^*$
		$\widehat{\alpha}^* = \frac{\alpha^* \cdot 10^{-3} \cdot \varepsilon}{k_{\mathrm{B}}}$
		$\widehat{\beta}^* = \frac{\beta^* \cdot 10^{21} \cdot \varepsilon}{\sigma^3}$
		$\widehat{\gamma}^* = \frac{\gamma^* \cdot 10^{-24} \cdot \sigma^3}{k_{\mathrm{B}}}$
		$\widehat{c}^*_v = \frac{3}{2} + c^*_{v,\mathrm{r}}$
		with $\frac{\varepsilon}{k_{\mathrm{B}}} = 119.76\,\mathrm{K}$, $\sigma = 3.405\,\mathrm{Å}$
McDonald and Singer[19]	$\widehat{T}^* = \frac{k_{\mathrm{B}}(T + 273.15\,\mathrm{K})}{\varepsilon}$	$\widehat{p}^* = Z \cdot \widehat{\rho}^* \cdot \widehat{T}^*$
[MCDSIN2]	$\widehat{\rho}^* = \left(\frac{v}{v^*}\right)^{-1}$	$\widehat{u}^*_{\mathrm{res}} = -\widehat{T}^* \cdot u^*_{\mathrm{r}}$
		$\widehat{c}^*_v = \frac{3}{2} + c^*_{v,\mathrm{r}}$
		with $\frac{\varepsilon}{\mathrm{k_B}} = 119.76\,\mathrm{K}$, $\sigma = 3.405\,\mathrm{Å}$
Barker et al.[167]	$\widehat{T}^* = T^*$	$\widehat{B} = \frac{2}{3}\pi \cdot B^*$
[BARLEOP]		$\widehat{C} = (\frac{2}{3}\pi)^2 \cdot C^*$
McDonald and Singer[49]	$\widehat{T}^* = T\frac{k_{\mathrm{B}}}{\varepsilon}$	$\widehat{p}^* = \frac{P \cdot 101.325 \cdot \sigma^3 \cdot 10^{-27}}{\varepsilon}$
[MCDSIN3]	$\widehat{\rho}^* = \frac{10^{-24} \cdot \sigma^3 \cdot N_{\mathrm{AV}}}{V}$	$\widehat{u}^*_{\mathrm{res}} = \frac{-u \cdot 4.184}{N_{\mathrm{AV}} \cdot \varepsilon}$
		with $\frac{\varepsilon}{k_{\mathrm{B}}} = 119.8\,\mathrm{K}$, $\sigma = 3.405\,\mathrm{Å}$
Adams[60]	$\widehat{T}^* = T^*$	$\widehat{c}^*_v = \frac{3}{2} + c^*_{v,\mathrm{r}}$
[ADAMS2]	$\widehat{\rho}^* = \rho^*$	$\widehat{\mu}^* = \widetilde{\mu}'$

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Authors & **[Acronym]**	**state point** T, ρ	**thermophysical** **properties**
		$\widehat{p}^* = p^*$
		$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
		$\widehat{\beta}^* = \widetilde{\beta}$
		$\Delta\widehat{h}^*_v = \Delta\widetilde{h}$
Sowers and Sandler[70]	$\widehat{T}^* = T^*$	$\widehat{p}^* = Z \cdot \widehat{\rho}^* \cdot \widehat{T}^*$
[SOWSAND]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
Shi and Johnson[120]	$\widehat{T}^* = T^*$	
[SHIJOHN]	$\widehat{\rho}^* = \rho^*$	
Morsali et al.[82]	$\widehat{T}^* = T^*$	$\widehat{\beta}^* = \kappa^*_{\mathrm{MD}}$
[MORSALI]	$\widehat{\rho}^* = \rho^*$	$\widehat{\gamma}^* = \gamma^*_{\mathrm{MD}}$
		$\widehat{p}^* = p^*$
Kolafa and Nezbeda[76]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[KOLNEZB]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
Lotfi et al.[71]	$\widehat{T}^* = T^*$	$\widehat{\beta}^* = \beta*$
[LOTVRAB]	$\widehat{\rho}^* = \rho^*$	$\widehat{p}^* = p^*$
		$\widehat{u}^*_{\mathrm{res}} = u^*_r$
		$\widehat{\Delta h}^*_v = h''^* - h'^*$
		$\widehat{\mu}^*_{\mathrm{res}} = (\widetilde{\mu} - \ln(\widehat{\rho}^*)) \cdot \widehat{T}^*$
Miyano[75]	$\widehat{T}^* = T^*$	$\widehat{p}^* = Z \cdot \widehat{\rho}^* \cdot \widehat{T}^*$
[MIYANO]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}} \cdot \widehat{T}^*$
Nicolas et al.[61]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[NICOLAS]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
		$\widehat{B} = B \cdot \frac{2\pi}{3}$
Saager and Fischer[69]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[SAAGFI]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$

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Authors & [Acronym]	state point T, ρ	thermophysical properties
Kofke[104]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = P$
[KOFKE]	$\widehat{\rho}^* = \rho^*$	$\Delta\widehat{h}_v^* = (u_\mathrm{l} - \frac{\widehat{p}_\mathrm{l}^*}{\widehat{\rho}_\mathrm{l}^*} + (-\widehat{u}_\mathrm{v} + \frac{\widehat{p}_\mathrm{v}^*}{\widehat{\rho}_\mathrm{v}^*}))$
Adams[58]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[ADAMS3]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}_\mathrm{res}^* = u_\mathrm{r}^*$
		$\widehat{\mu}_\mathrm{res}^* = \mu_\mathrm{r}^*$
		$\Delta\widehat{h}_v^* = \Delta h_v^*$
		$\widehat{p}_v^* = p_v^*$
Mecke et al.[78]	$\widehat{T}^* = T^*$	$\widehat{u}_\mathrm{res}^* = u_\mathrm{r}^*$
[MECK]	$\widehat{\rho}^* = \rho^*$	$\widehat{p}^* = p^*$
Potoff and Panagiotopoulos[116]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = \gamma^*$
[POTPAN2]	$\widehat{\rho}^* = \rho^*$	
Kolafa et al.[74]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[KOLVOR]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}_\mathrm{res}^* = u_\mathrm{r}^*$
		$\widehat{\mu}_\mathrm{res}^* = \widehat{T}^* \cdot \mu_\mathrm{r}^*$
Emampour et al.[157]	$\widehat{T}^* = T^*$	$\widehat{\Gamma}^* = \Gamma^*$
[EMAM]	$\widehat{\rho}^* = \rho^*$	
Agrawal and Kofke[106]	$\widehat{T}^* = \frac{1}{T^*}$	$\widehat{p}_v^* = 10^{-3} \cdot p^*$
[AGRKOF]	$\widehat{\rho}_\mathrm{l}^* = \rho_\mathrm{l}^*$	$\Delta\widehat{h}_v^* = (-u_\mathrm{g}^* + \frac{\widehat{p}^*}{\widehat{\rho}_\mathrm{v}^*} + u_\mathrm{l}^* - \frac{\widehat{p}^*}{\widehat{\rho}_\mathrm{l}^*})$
	$\widehat{\rho}_\mathrm{v}^* = \rho_\mathrm{g}^* \cdot 10^{-3}$	
Lustig[77]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[LUSTIG]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}_\mathrm{res}^* = u_\mathrm{r}^*$
		$\widehat{\beta}^* = \beta^*$
		$\widehat{\mu}_\mathrm{res}^* = \mu_\mathrm{r}^*$
		$\widehat{\gamma}^* = \gamma^*$
Boda et al.[154]	$\widehat{T}^* = T^*$	$\widehat{c}_v^* = \frac{3}{2} + c_{v,\mathrm{r}}^*$

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Authors & [Acronym]	state point T, ρ	thermophysical properties
[BODA]	$\widehat{\rho}^* = \rho^*$	$\widehat{c}_p^* = c_{p,\mathrm{r}}^* + 1.5$
Weeks et al.[53] [WEECKCHA2]	$\widehat{T}^* = T^*$ $\widehat{\rho}^* = \rho^*$	$\widehat{u}_{\mathrm{res}}^* = -u_{\mathrm{r}}$ $\widehat{a}_{\mathrm{res},00}^* = -A_{\mathrm{r},00}$ $\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot \frac{\beta p}{\rho}$
Verlet and Levesque[46] [VERLEV]	$\widehat{T}^* = T^*$ $\widehat{\rho}^* = \rho^*$	$\widehat{u}_{\mathrm{res}}^* = u_{\mathrm{r}}^*$ $\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot \frac{\beta p}{\rho}$
Mecke et al.[109] [MECKWIN]	$\widehat{T}^* = T^*$ $\widehat{\rho}^* = \rho^*$	$\widehat{\gamma}^* = \gamma^*$
Toxvaerd and Praestgaard[52] [TOXPRA]	$\widehat{T}^* = T^*$ $\widehat{\rho}^* = \rho^*$	$\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot Z$
Street et al.[56] [STRRAV]	$\widehat{T}^* = T^*$ $\widehat{\rho}^* = \rho^*$	$\widehat{p}^* = p^*$ $\widehat{u}_{\mathrm{res}}^* = u_{\mathrm{r}}^*$
Carley[59] [CARL]	$\widehat{T}^* = T^*$ $\widehat{\rho}^* = \rho^*$	$\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot Z$
Schofield[55] [SCHOF]	$\widehat{T}^* = T^*$ $\widehat{\rho}^* = \rho^*$	$\widehat{p}^* = \rho^* \cdot \widehat{T}^* \frac{p_f}{n \cdot k_{\mathrm{B}} \cdot T^*}$
McDonald and Woodcock[51] [MCDWOO]	$\widehat{T}^* = \frac{T \cdot k_{\mathrm{B}}}{\varepsilon}$ $\widehat{\rho}^* = \frac{\rho \cdot N_{\mathrm{AV}} \cdot \sigma^3 \cdot 10^{-24}}{M}$	$\widehat{p}^* = \widehat{\rho}^* \cdot \widehat{T}^* \cdot Z$ $u_{\mathrm{res}}^* = u^* \cdot \widehat{T}^*$ $\frac{\varepsilon}{k_{\mathrm{B}}} = 117.2\,\mathrm{K},\ \sigma = 3.405\,\mathrm{Å}$ $M = 39.948\,\frac{\mathrm{g}}{\mathrm{mol}}$
Roccatano et al.[79] [ROCAMA]	$\widehat{T}^* = T^*$ $\widehat{\rho}^* = \rho^*$	$\widehat{c}_v^* = \frac{3}{2} + c_{v,\mathrm{r}}^*$ $\widehat{u}_{\mathrm{res}}^* = u_{\mathrm{r}}^*$ $\widehat{p}^* = p^*$
Lustig[84] [LUSTIG2]	$\widehat{T}^* = T^*$ $\widehat{\rho}^* = \rho^*$	$\widehat{c}_p^* = c_p^*$ $\widehat{\mu}_{\mathrm{JT}}^* = \mu_{\mathrm{JT}}^*$

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Authors & [Acronym]	**state point** T, ρ	**thermophysical properties**
		$\widehat{p}^* = p^*$
		$\widehat{w}^* = w^*$
Wood[47]	$\widehat{T}^* = \theta$	$\widehat{p}^* = Z \cdot \widehat{\rho}^* \cdot \widehat{T}^*$
[WOOD]	$\widehat{\rho}^* = \frac{1}{\tau}$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}} \cdot \theta$
Martin and Siepmann[113]	$\widehat{T^*} = \frac{T \cdot k_{\mathrm{B}}}{\varepsilon}$	$\widehat{p}^*_v = \frac{p_v \cdot \sigma^3 \cdot 10^{-27}}{\varepsilon}$
[MARSIE]	$\widehat{\rho^*} = \frac{\rho \cdot N_{\mathrm{AV}} \cdot \sigma^3 \cdot 10^{-24}}{M}$	
		with $\frac{\varepsilon}{k_{\mathrm{B}}} = 147.9\,\mathrm{K}$, $\sigma = 3.73\,\mathrm{Å}$,
		$M = 16.04\,\frac{\mathrm{g}}{\mathrm{mol}}$
Fickett and Wood[44]	$\widehat{T}^* = \frac{T \cdot k_{\mathrm{B}}}{\varepsilon}$	$\widehat{p}^* = \frac{p \cdot \sigma^3 \cdot 10^{-22}}{\varepsilon}$
[FICWOO]	$\widehat{\rho}^* = \frac{N_{\mathrm{AV}} \cdot \sigma^3 \cdot 10^{-24}}{v}$	
		with $\frac{\varepsilon}{k_{\mathrm{B}}} = 119.3\,\mathrm{K}$, $\sigma = 3.833\,\mathrm{Å}$
Shaul et al.[169]	$\widehat{T}^* = T^*$	$\widehat{B}^* = B_2 \cdot \sigma^{-3}$
[SHASCH]		$\widehat{C}^* = B_3 \cdot \sigma^{-6}$
Bird et al.[165]	$\widehat{T}^* = T^*$	$\widehat{C}^* = (\frac{2}{3}\pi)^2 \cdot C^{(0)}$
[BIRSPO]		
Hirschfelder et al.[166]	$\widehat{T}^* = T^*$	$\widehat{B}^* = B^* \cdot \frac{3}{2\pi}$
[HIRCUR]		$\widehat{C}^* = C^* \cdot (\frac{3}{2\pi})^2$
Baidakov et al.[117]	$\widehat{T}^* = T^*$	$\widehat{p}^*_v = \frac{p^*_v}{10}$
[BAIDAKO]	$\widehat{\rho}^* = \rho^*$	$\widehat{\gamma}^* = \gamma^*$
Baidakov et al.[83]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[BAIDAKO2]	$\widehat{\rho}^* = \rho^*$	$\widehat{c}^*_v = c^*_v$
		$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
Linhart et al.[81]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[LINHART]	$\widehat{\rho}^* = \rho^*$	
Lafitte et al.[11]	$\widehat{T}^* = T^*$	$\widehat{a}^*_1 = A^*_1$

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Authors & **[Acronym]**	**state point** T, ρ	**thermophysical properties**
[LAFITTE]	$\widehat{\rho^*} = \rho^*$	$\widehat{a}_2^* = A_2^*$
		$\widehat{a}_3^* = A_3^*$
Data was digitalized from the corresponding plots from Ref.[11]		
Lucas[65]	$\widehat{T}^* = T^*$	$\widehat{p}^* = Z \cdot \widehat{\rho}^* \cdot \widehat{T}^*$
[LUCAS]	$\widehat{\rho^*} = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = \frac{E}{R \cdot T} \cdot \widehat{T}^*$
Betancourt-Cárdenas et al.[130]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[BETANCOU]	$\widehat{\rho}^* = \rho^*$	$\widehat{a}_2 = A_2, \quad \widehat{a}_1 = A_1$
		$\Delta \widehat{h}_v^* = u_{\mathrm{v}}^* + \frac{\widehat{p}_{\mathrm{v}}^*}{\widehat{\rho}_{\mathrm{v}}^*} - u_{\mathrm{l}}^* - \frac{\widehat{p}_{\mathrm{l}}^*}{\widehat{\rho}_{\mathrm{l}}^*}$
Janeček et al.[135]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = p_v^*$
[JANECEK]	$\widehat{\rho}^* = \rho^*$	$\Delta \widehat{h}_v^* = \Delta h_v^*$
		$\widehat{\gamma}^* = \gamma^*$
The VLE data from the *inhomogeneous simulations* were digitalized from the corresponding plots from Ref.[135] In this work the *inhomogeneous simulations*-data from *Janeček et al.*[135] is referred to as data from Ref.[135] and [JANECEK]. For the *GEMC* results from the same publication see [PRIVJANEC].		
Guo et al.[111]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = \gamma^*$
[GUO]	$\widehat{\rho}^* = \rho^*$	
Surface tension data was digitalized from the corresponding plots from Ref.[111]		
Lee et al.[98]	$\widehat{T}^* = \frac{T \cdot k_{\mathrm{B}}}{\varepsilon}$	$\widehat{\gamma}^* = 0.001 \cdot \gamma \sigma^2 \varepsilon^{-1}$
[LEE]	$\widehat{\rho}^* = \rho^*$	
		with $\frac{\varepsilon}{k_{\mathrm{B}}} = 119.4\,\mathrm{K}$, $\sigma = 3.4\,\mathrm{\AA}$
Werth et al.[137]	$\widehat{T}^* = T^*$	$\Delta \widehat{h}_v^* = \Delta h_v *$
[WERTH]	$\widehat{\rho}^* = \rho^*$	$\widehat{p}_v^* = p_v^*$
		$\widehat{\gamma}^* = \gamma^*$
Stephan and Hasse[138]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = p_v^*$

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Authors & [Acronym]	**state point** T, ρ	**thermophysical properties**
[STEPHAN2]	$\widehat{\rho}^* = \rho^*$	
Nijmeijer et al.[102]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = \gamma^*$
[NIJMEIJ]	$\widehat{\rho}^* = \rho^*$	
Errington[125]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = p_v^*$
[ERRING]	$\widehat{\rho}^* = \rho^*$	$\widehat{\gamma}^* = \gamma^*$
Baidakov et al.[129]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = p_v^*$
[BAIDAKOV1]	$\widehat{\rho}^* = \rho^*$	$\widehat{\gamma}^* = \gamma^*$
Janeček[131]	$\widehat{T}^* = T^*$	$\Delta\widehat{h}_v^* = \Delta h_v *$
[JANECE]	$\widehat{\rho}^* = \rho^*$	$\widehat{p}_v^* = p_v^*$
		$\widehat{\gamma}^* = \gamma^*$
Martinez-Ruiz et al.[134]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = p_v^*$
[MARTINEZ]	$\widehat{\rho}^* = \rho^*$	$\widehat{\gamma}^* = \gamma^*$
Chen et al.[24]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = \gamma^*$
[CHEN]	$\widehat{\rho}^* = \rho^*$	
Galliero et al.[132]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = \gamma^*$
[GALLIER]	$\widehat{\rho}^* = \rho^*$	
Trokhymchuk and Alejandre[114]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = p_v^*$
[TROK]	$\widehat{\rho}^* = \rho^*$	$\widehat{\gamma}^* = \gamma^*$
Anisimov et al.[115]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = p_v^* \cdot 10^{-3}$
[ANISIMOV]	$\widehat{\rho}^* = \rho^*$	$\widehat{\gamma}^* = \gamma^*$
Guo and Lu[112]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = \gamma^*$
[GUOLU]	$\widehat{\rho}^* = \rho^*$	
Mausbach et al.[159]	$\widehat{T}^* = T^*$	$\widehat{\Gamma}^* = \Gamma^*$
[MAUSVRAB]	$\widehat{\rho}^* = \rho^*$	
Köster et al.[91]	$\widehat{T}^* = T^*$	$\widehat{a}_{\mathrm{res},01}^* = A_{\mathrm{r},01}^*$

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Authors & [Acronym]	state point T, ρ	thermophysical properties
[KOESTER]	$\widehat{\rho}^* = \rho^*$	$\widehat{\tilde{a}}^*_{\mathrm{res},11} = A^*_{\mathrm{r},11}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},10} = A^*_{\mathrm{r},10}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},20} = A^*_{\mathrm{r},20}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},02} = A^*_{\mathrm{r},02}$
Köster et al.[91,92]	$\widehat{T}^* = T^*$	$\widehat{\tilde{a}}^*_{\mathrm{res},00} = A^*_{\mathrm{r},00}$
[KOESTERPRIVCOM]	$\widehat{\rho}^* = \rho^*$	$\widehat{\tilde{a}}^*_{\mathrm{res},01} = A^*_{\mathrm{r},01}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},10} = A^*_{\mathrm{r},10}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},11} = A^*_{\mathrm{r},11}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},02} = A^*_{\mathrm{r},02}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},20} = A^*_{\mathrm{r},20}$
Some of the numerical values from Ref.[91] were not included in the corresponding supplementary material. This data was made available by the authors and is included in the database as [KOESTERPRIVCOM] and referred to as data from Ref.[91,92]		
Yao et al.[63]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[YAO]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = -U^*/N$
		$\widehat{\mu}^*_{\mathrm{res}} = -\mu^* - \ln(\widehat{\rho}^*) \cdot T^*$
Baidakov et al.[123]	$\widehat{T}^* = T^*$	$\widehat{\rho}^* = \rho^*$
[BAIDAKOV2]	$\widehat{\rho}^* = \rho^*$	$\widehat{\gamma}^* = \gamma^*$
Data was digitalized from the corresponding plots from Ref.[123]		
Hong and Jhon[163]	$\widehat{T}^* = T^*$	$\widehat{\tilde{a}}^*_{\mathrm{res},00} = -A^*_{\mathrm{res},00}$
[SEUNGMU]	$\widehat{\rho}^* = \rho^*$	
Torrie and Valleau[96]	$\widehat{T}^* = T^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
[TORVAL]	$\widehat{\rho}^* = N/V^*$	$\widehat{\tilde{a}}^*_{\mathrm{res},00} = (\frac{A_c}{N \cdot \varepsilon}) \cdot \frac{1}{\widehat{T}^*} - \ln(\widehat{\rho}^*) + 1$
Schultz and Kofke[95]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$

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Authors & [Acronym]	state point T, ρ	thermophysical properties
[SCHULTZKOFKE]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
van Westen and Gross[10]	$\widehat{T}^* = T^*$	$\widehat{a}^*_1 = A^*_1$
[WESTGROSS]	$\widehat{\rho}^* = \rho^*$	$\widehat{a}^*_2 = A^*_2$
		$\widehat{a}^*_3 = A^*_3$
this work	$\widehat{T}^* = T^*$	$\widehat{\tilde{a}}^*_{\mathrm{res},00} = \tilde{a}^*_{\mathrm{res},00}$
[STEPHANTHIS]	$\widehat{\rho}^* = \rho^*$	$\widehat{\tilde{a}}^*_{\mathrm{res},01} = \tilde{a}^*_{\mathrm{res},01}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},10} = \tilde{a}^*_{\mathrm{res},10}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},11} = \tilde{a}^*_{\mathrm{res},11}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},02} = \tilde{a}^*_{\mathrm{res},02}$
		$\widehat{\tilde{a}}^*_{\mathrm{res},20} = \tilde{a}^*_{\mathrm{res},20}$
		$p^*_v = p^*_v$
		$\Delta h^*_v = \Delta h^*_v$
Errington[126,127]	$\widehat{T}^* = T^*$	$\widehat{p}^*_v = p^*_v$
[ERRING2]	$\widehat{\rho}^* = \rho^*$	
The data listed as [ERRING2] was forwarded by J. Errington.[127] Please note, that two websites provide numerical values for the LJ VLE.[215,216] The website can be understood in a way that the numeric values might be those of Ref.,[126] cf. Ref.[10] The numeric values from[215,216] are however dissimilar than those from.[126,127]		
Janeček et al.[135,136]	$\widehat{T}^* = T^*$	$\Delta\widehat{h}^*_v = \Delta h^*_v$
[PRIVJANEC]	$\widehat{\rho}^* = \rho^*$	$\widehat{p}^*_v = p^*_v$
The numeric values of the VLE data from the *GEMC simulations* from Ref.[135] were made available by J. Janeček[136] and are listed in the database as [PRIVJANEC].		
Okumura and Yonezawa[118,119]	$\widehat{T}^* = T^*$	$\widehat{p}^*_v = p^*_v$
[PRIVOKU]	$\widehat{\rho}^* = \rho^*$	
Kioupis et al.[124]	$\widehat{T}^* = T^*$	$\widehat{p}^*_v = p_{\mathrm{sat}}$
[KIOUPIS]	$\widehat{\rho}^* = \rho$	$\Delta\widehat{h}^*_v = H_{\mathrm{vap}} - H_{\mathrm{liq}}$

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Authors & **[Acronym]**	**state point** T, ρ	**thermophysical** **properties**
Okumura and Yonezawa[121,122]	$\widehat{T}^* = T^*$	$\widehat{p}^*_v = p^*_v$
[PRIVOKU2]	$\widehat{\rho}^* = \rho^*$	
Mick et al.[23]	$\widehat{T}^* = T^*$	$\widehat{p^*}_v = p^*_v$
[MICK]	$\widehat{\rho}^* = \rho^*$	$\Delta\widehat{h}^*_v = u^*_v + \frac{p^*}{\widehat{\rho}^*_v} - u^*_l - \frac{p^*}{\widehat{\rho}^*_l}$
Ustinov[93,94]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[PRIVUSTINOV]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
		$\widehat{\mu}^*_{\mathrm{res}} = \mu^*$
Hong and Jang[164]	$\widehat{T}^* = T^*$	$\widehat{\widehat{a}}^*_{\mathrm{res},00} = -A^{\mathrm{ex}}/Nk_{\mathrm{B}}T$
[HONG]	$\widehat{\rho}^* = \rho^*$	
Giaquinta et al.[72]	$\widehat{T}^* = T^*$	$\widehat{p}^* = \frac{\beta P}{\rho} \cdot \widehat{\rho}^* \cdot \widehat{T}^*$
[GIAQUI]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
Cuadros et al.[162]	$\widehat{T}^* = T^*$	$\widehat{\widehat{a}}^*_{\mathrm{res},00} = \frac{A_{\mathrm{r},00}}{\widehat{T}^*}$
[CUADROS]	$\widehat{\rho}^* = \rho^*$	
Adachi et al.[67]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[ADACHI]	$\widehat{\rho}^* = \rho^*$	
Baranyai et al.[68]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p^*$
[BARANY]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^*_{\mathrm{res}} = u^*_{\mathrm{r}}$
		$\widehat{\widehat{a}}^*_{\mathrm{res},00} = \frac{A^{\mathrm{ex}}/N}{\widehat{T}^*}$
Powles et al.[64]	$\widehat{T}^* = T^*$	$\widehat{p}^* = p - 1.09 \cdot (\widehat{\rho}^*)^2$
[POWLES]	$\widehat{\rho}^* = \rho^*$	$\widehat{\mu}^*_{\mathrm{res}} = \mu_1 - \widehat{T}^* \cdot \ln(\widehat{\rho}^*)$
		$+ \frac{3}{2}\,\widehat{T}^* \cdot \ln(\widehat{T}^*) - 1.86\,\widehat{\rho}^*$
Han[161]	$\widehat{T}^* = T^*$	$\widehat{\mu}^*_{\mathrm{res}} = \widehat{T}^* \cdot \mu^*_{\mathrm{r}}$
[HAN]	$\widehat{\rho}^* = \rho^*$	
Holcomb et al.[105]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = \gamma^*$
[HOLCOMB]	$\widehat{\rho}^* = \widehat{\rho}^*$	

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Authors & [Acronym]	**state point** T, ρ	**thermophysical properties**
Stoll et al.[128]	$\widehat{T}^* = \frac{T^*}{4}$	$\widehat{p}_v^* = \frac{1}{4} p_v^*$
[STOLL]	$\widehat{\rho}^* = \widehat{\rho}^*$	$\Delta \widehat{h}_v^* = \frac{h_{v,vap} - h_{v,liq}}{4}$
Deiters and Neumaier[43,97]	$\widehat{T}^* = \frac{T \cdot k_\mathrm{B}}{\varepsilon}$	$\widehat{p}^* = \frac{p^* \cdot 10^{-24} \cdot \sigma^3}{(\varepsilon / k_\mathrm{B}) \cdot k_\mathrm{B}}$
[DEINEU]	$\widehat{\rho}^* = \frac{10^{-24} \cdot N_\mathrm{AV} \cdot \sigma^3}{V_M}$	$\widehat{u}_\mathrm{res}^* = \frac{u_\mathrm{m}}{(\varepsilon / k_\mathrm{B}) \cdot k_\mathrm{B} \cdot N_\mathrm{AV}}$
		with $\frac{\varepsilon}{k_\mathrm{B}} = 119.8\,\mathrm{K}$, $\sigma = 3.405\,\mathrm{\AA}$
Sun and Teja[168]	$\widehat{T}^* = T^*$	$\widehat{B}^* = \frac{2}{3}\pi \cdot B_2^*$
[SUNTEJA]		$\widehat{C}^* = (\frac{2}{3}\pi)^2 \cdot B_3^*$
Sadus and Prausnitz[108]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = P^*$
[SADUS]	$\widehat{\rho}^* = \rho^*$	$\Delta \widehat{h}_v^* = (E_\mathrm{v}^* + \frac{\widehat{p}_\mathrm{v}^*}{\widehat{\rho}_\mathrm{v}^*} - (E_\mathrm{l}^* + \frac{\widehat{p}_\mathrm{l}^*}{\widehat{\rho}_\mathrm{l}^*}))$
Yigzawe and Sadus[87]	$\widehat{T}^* = \varphi \cdot 1.312$	$\widehat{p}^* = p^*$
[YIGSAD]	$\widehat{\rho}^* = \rho^*$	
Yigzawe[86]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = p^*$
[YIGZAWE]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^* = u^* - \frac{3}{2}\widehat{T}^*$
		$\widehat{c}_p^* = C_p^*$
		$\widehat{c}_v^* = C_v^*$
		$\widehat{\alpha}^* = \alpha_\mathrm{P}^*$
		$\widehat{\beta}^* = \beta_\mathrm{T}^*$
		$\widehat{\gamma}^* = \gamma_\mathrm{V}^*$
		$\widehat{\mu}_\mathrm{JT}^* = \mu_\mathrm{JT}^*$
		$\widehat{w}^* = w_0^*$
Mairhofer and Sadus[88,89]	$\widehat{T}^* = T^*$	$\widehat{p}_v^* = p^*$
[PRIVMAI]	$\widehat{\rho}^* = \rho^*$	$\widehat{u}^* = u^* - \frac{3}{2}\widehat{T}^*$
		$\widehat{c}_p^* = C_p^*$
		$\widehat{c}_v^* = C_v^*$
		$\widehat{\beta}^* = \beta_\mathrm{T}^*$

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Authors & [Acronym]	**state point** T, ρ	**thermophysical properties**
		$\widehat{\gamma}^* = \gamma^*$
		$\widehat{\mu}^*_{\mathrm{JT}} = \mu^*_{\mathrm{JT}}$
		$\widehat{w}^* = w^*_0$
Plačkov and Sadus[110]	$\widehat{T}^* = T^*$	$\widehat{p}^*_v = P^*$
[PLACKOV]	$\widehat{\rho}^* = \rho^*$	$\Delta\widehat{h}^*_v = (E^*_{\mathrm{v}} + \frac{\widehat{p}^*_{\mathrm{v}}}{\widehat{\rho}^*_{\mathrm{v}}} - (E^*_{\mathrm{l}} + \frac{\widehat{p}^*_{\mathrm{l}}}{\widehat{\rho}^*_{\mathrm{l}}}))$
Sadus[133]	$\widehat{T}^* = T^*$	$\widehat{p}^*_v = p^*$
[SADUS2]		
Chapela et al.[99]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = \gamma^*$
[CHAPELA]		
Shen et al.[141]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = \gamma^*$
[SHEN]		
Werth et al.[142]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = \gamma^*$
[WERHOR]		
Miyazaki et al.[139]	$\widehat{T}^* = T^*$	$\widehat{\gamma}^* = 0.001 \cdot \gamma\sigma^2\varepsilon^{-1}$
[MIYAZ]		
		with $\frac{\varepsilon}{k_{\mathrm{B}}} = 119.8\,\mathrm{K}$, $\sigma = 3.405\,\mathrm{\AA}$

Details on the assessment of homogeneous states data

Fig. S1 shows the results of the EOS test on the homogeneous state points as the percentage of the overall confirmed data as a function of the parameter $P_{\max}$. The chosen value of $P_{\max} = 4$ is indicated, which entails approximately 90% confirmed data. For smaller $P_{\max}$ values, the EOS test becomes more stringent as more data points are characterized as outliers. For larger $P_{\max}$ values, the EOS test becomes more lenient (i.e. more conservative) and less data points are identified as outliers. Evidently, the EOS test converges for large P_{max} values to approximately $N_{\mathrm{conf}} = 98\%$, which means that these 2% of all homogeneous data are particularly gross outliers.

Details on the calculation of thermophysical properties by the *Lustig*-formalism

The *Lustig* formalism in combination with Widom's test particle insertion method,[176] as implemented in the simulation package *ms*2,[177] provides the Helmholtz energy and its derivatives with respect to the density and the inverse temperature simultaneously from a single simulation run. The Helmholtz energy per particle $a = A/N$ is formally split into an ideal gas contribution (superscript o) and a residual contribution (superscript res), i.e. $a = a^{\mathrm{o}} + a^{\mathrm{res}}$. The following notation is used for the derivatives of the Helmholtz energy $\tilde{a} = a/T$ with respect to inverse temperature and density

$$\tilde{a}_{nm} = \tilde{a}^{\mathrm{o}}_{\mathrm{nm}} + \tilde{a}^{\mathrm{res}}_{\mathrm{nm}} = (1/T)^n \, \rho^m \, \frac{\partial^{n+m}(\tilde{a}^{\mathrm{o}} + \tilde{a}^{\mathrm{res}})}{\partial (1/T)^n \, \partial \rho}, \quad (1)$$

where only $n, m = 0, 1, 2$ and were considered here. The numerical values of the $\tilde{a}_{nm}$ obtained in the studies of Refs.[90–92] and from this work are included in the database, as such are the primary simulation data. The relations used for the computation of thermodynamic properties from the sampled $\tilde{a}_{nm}$ values are as follows:

entropic properties

Gibbs energy $$g = h - Ts = T(1 + \tilde{a}^{\mathrm{o}}_{00} + \tilde{a}^{\mathrm{res}}_{00} + \tilde{a}^{\mathrm{res}}_{01}) \quad (2)$$

thermal properties

pressure $$p = -\left(\frac{\partial a}{\partial v}\right)_T = \rho T \, (1 + \tilde{a}^{\mathrm{res}}_{01}) \quad (3)$$

thermal pressure coefficient $$\gamma = \left(\frac{\partial p}{\partial T}\right)_\rho = \rho(1 + \tilde{a}_{01}^{\text{res}} - \tilde{a}_{11}^{\text{res}}) \quad (4)$$

isothermal compressibility $$\beta = \left(\rho \frac{\partial p}{\partial \rho}\right)_T^{-1} = \frac{1}{\rho T(1 + 2\tilde{a}_{01}^{\text{res}} + \tilde{a}_{02}^{\text{res}})} \quad (5)$$

thermal expansion coefficient $$\alpha = \beta\gamma = \frac{\left(\frac{\partial p}{\partial T}\right)_\rho}{\rho\left(\frac{\partial p}{\partial \rho}\right)_T} = \frac{1 + \tilde{a}_{01}^{\text{res}} - \tilde{a}_{11}^{\text{res}}}{T(1 + 2\tilde{a}_{01}^{\text{res}} + \tilde{a}_{02}^{\text{res}})} \quad (6)$$

caloric properties

internal energy $$u = a + Ts = T(\tilde{a}_{10}^{0} + \tilde{a}_{10}^{\text{res}}) \quad (7)$$

$$u_{\text{res}} = a_{\text{res}} + Ts_{\text{res}} = T\tilde{a}_{10}^{\text{res}} \quad (8)$$

enthalpy $$h = u + pv = T(1 + \tilde{a}_{10}^{\text{o}} + \tilde{a}_{10}^{\text{res}} + \tilde{a}_{01}^{\text{res}}) \quad (9)$$

isobaric heat capacity $$c_p = \left(\frac{\partial h}{\partial T}\right)_p = -(\tilde{a}_{20}^{\text{o}} + \tilde{a}_{20}^{\text{res}}) + \frac{(1 + \tilde{a}_{01}^{\text{res}} - \tilde{a}_{11}^{\text{res}})^2}{1 + 2\tilde{a}_{01}^{\text{res}} + \tilde{a}_{02}^{\text{res}}} \quad (10)$$

isochoric heat capacity $$c_v = \left(\frac{\partial u}{\partial T}\right)_v = -(\tilde{a}^{\mathrm{o}}_{20} + \tilde{a}^{\mathrm{res}}_{20}) \tag{11}$$

speed of sound $$w = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \left(T(1 + 2\tilde{a}^{\mathrm{res}}_{01} + \tilde{a}^{\mathrm{res}}_{02}) - \frac{(1 + \tilde{a}^{\mathrm{res}}_{01} - \tilde{a}^{\mathrm{res}}_{11})^2}{\tilde{a}^{\mathrm{o}}_{20} + \tilde{a}^{\mathrm{res}}_{20}}\right)^{0.5} \tag{12}$$

Joule-Thomson coefficient $$\mu_{\mathrm{JT}} = \left(\frac{\partial T}{\partial p}\right)_h \tag{13}$$

$$= \rho^{-1} \frac{-(\tilde{a}^{\mathrm{res}}_{01} + \tilde{a}^{\mathrm{res}}_{02} + \tilde{a}^{\mathrm{res}}_{11})}{(1 + \tilde{a}^{\mathrm{res}}_{01} - \tilde{a}^{\mathrm{res}}_{11})^2 - (\tilde{a}^{\mathrm{o}}_{20} + \tilde{a}^{\mathrm{res}}_{20})(1 + 2\tilde{a}^{\mathrm{res}}_{01} + \tilde{a}^{\mathrm{res}}_{02})}$$

Grüneisen coefficient $$\Gamma = \frac{\left(\frac{\partial p}{\partial T}\right)_\rho}{\rho\, c_v} = \frac{1 + \tilde{a}^{\mathrm{res}}_{01} - \tilde{a}^{\mathrm{res}}_{11}}{-\tilde{a}^{\mathrm{o}}_{20} - \tilde{a}^{\mathrm{res}}_{20}} \tag{14}$$

Details on the assessment of VLE bulk data

The results of the three VLE tests for all data sets (both confirmed and discarded) are shown in Figs. S2, S3, and S4 for the sake of completeness. Fig. S2 of the supplementary material shows the results of the compressibility factor test for all VLE data, Fig. S3 shows the results of the Clausius-Clapeyron test for all VLE data, and Fig. S4 shows the deviations from all VLE data and the base correlations (6) - (9).

Data sets that were discarded according the criteria for the compressibility factor test (cf. Fig. S2) outlined in the main part of this work are those from *Adams*,[58] *Adams*,[60] *Anisimov* *et al.*,[115] *Baidakov et al.*,[117] *Baidakov et al.*,[129] *Betancourt-Cárdenas et al.*,[130] *Kioupis et al.*,[124] *Martin and Siepmann*,[113] *Panagiotopoulos*,[100] *Panagiotopoulos et al.*,[101] *Smit and Frenkel*,[103] and *Trokhymchuk and Alejandre.*[114]

For the data sets from the literature that report all VLE properties required for the Clausius-Clapeyron test, the RHS of Eq. (10) was computed and shown in Fig. S3 for comparison. Large deviations from the base correlation and the most precise data sets (Refs.[23,71,135,136] and this work) were found for the data of *Adams*,[58] *Adams*,[60] *Kioupis et al.*,[124] *Betancourt-Cárdenas et al.*,[130] *Panagiotopoulos*,[100] *Panagiotopoulos et al.*,[101] and *Smit and Frenkel.*[103] According the criteria outlined in the main part of this work, these data sets were discarded.

Fig. S4 shows the deviation plots for each VLE property (p^s, ρ', ρ'', and Δh_v) for all VLE data sets considered in this work. The following data sets contain two or more data points with deviations larger than 5%, i.e. are out of the range of Fig. S4: *Adams*,[58] *Adams*,[60] *Anisimov et al.*,[115] *Baidakov et al.*,[117] *Baidakov et al.*,[129] *Baidakov et al.*,[123] *Betancourt-Cárdenas et al.*,[130] *Guo et al.*,[111] *Guo and Lu*,[112] *Galliero et al.*,[132] *Hunter and Reinhardt*,[107] *Holcomb et al.*,[105] *Janeček*,[131] *Kioupis et al.*,[124] *Kofke*,[104] *Lee et al.*,[98] *Martin and Siepmann*,[113] *Mecke et al.*,[109] *Okumura and Yonezawa*,[118,119] *Panagiotopoulos*,[100] *Panagiotopoulos et al.*,[101] *Potoff and Panagiotopoulos*,[197] *Smit and Frenkel*,[103] and *Trokhymchuk and Alejandre.*[114] These pronounced deviations were found in most cases for the vapor pressure and the saturated vapor density. Deviations of data points that exceed 5% in the saturated liquid density or the enthalpy of vaporization were only found for the data from *Panagiotopoulos*,[100] *Smit and Frenkel*,[103] *Kofke*,[104] *Kioupis et al.*,[124] *Hunter and Reinhardt*,[107] *Mecke et al.*,[109] and *Lee et al.*[98] Data sets exhibiting particularly large deviations from Eqs. (6) - (9) at multiple state points are those from *Anisimov et al.*,[115] *Baidakov et al.*,[117] *Baidakov et al.*,[129] *Galliero et al.*,[132] *Hunter and Reinhardt*,[107] *Kioupis et al.*,[124] *Lee et al.*,[98] *Panagiotopoulos*,[100] and *Trokhymchuk and Alejandre.*[114] To avoid visual clutter, these out-of-range data points are not shown in Fig. S4. This confirms the findings from the compressibility factor and the Clausius-Clapeyron tests where these data sets could be applied.

The data sets of *Hunter and Reinhardt*,[107] *Potoff and Panagiotopoulos*,[197] *Shi and Johnson*[120] (only saturated densities reported) show small, but distinct systematic deviations to the base correlation and the seven most precise data sets.

Details on the assessment of VLE interfacial data

Fig. S5 shows the surface tension of all considered data in this work. The surface tension results reported by *Trokhymchuk and Alejandre*[114] and the MC results of *Galliero et al.*[132] are slightly but noticeably below the mutually best agreeing data sets. The data of *Anisimov et al.*[115] show large deviations, which is likely a result of the employed LJ potential version.

The surface tension data of *Potoff and Panagiotopoulos*[116] shows distinct deviations from the above mentioned data of best mutual agreement – especially close to the critical point. The same was found for the saturated densities data of *Potoff and Panagiotopoulos*[116]. This is in line with the relatively low critical temperature reported by Ref..[116]

Table S4 summarizes the identified outliers in the data sets that were identified to be the best VLE data sets: *Errington*,[126,127] *Janeček et al.*,[135,136] *Lotfi et al.*,[71] *Mick et al.*,[23] *Okumura and Yonezawa*,[121,122] and this work.

Table S3 summarizes the results for the vapor-liquid equilibrium data obtained in this work using the Grand Equilibrium method[179] as implemented in *ms*2.[177]

Table S3: Simulation results for the VLE data set obtained in this work. The columns are from left to right: vapor pressure, saturated liquid density, saturated vapor density, and the enthalpy of vaporization. The numbers in parentheses indicate the uncertainties of the last decimal digits.

T	p^s	ρ'	ρ''	Δh_v
0.69	0.001172(24)	0.847111(1)	0.001729(35)	6.766422(34)
0.7	0.001343(25)	0.8427(1)	0.001956(36)	6.762403(39)
0.72	0.001784(28)	0.834385(1)	0.002538(39)	6.652809(43)
0.74	0.002319(29)	0.825751(1)	0.003227(40)	6.641588(48)
0.76	0.002932(32)	0.817195(2)	0.003994(44)	6.528674(58)
0.78	0.003689(40)	0.8083(1)	0.004929(54)	6.513863(71)
0.8	0.004649(44)	0.799470(2)	0.006103(57)	6.395171(72)
0.82	0.005608(44)	0.7903(1)	0.007233(57)	6.278050(94)
0.84	0.006872(44)	0.7812(1)	0.008730(55)	6.25512(12)
0.86	0.008299(53)	0.7718(1)	0.010397(66)	6.13070(14)
0.88	0.009902(63)	0.7623(1)	0.012248(78)	6.10391(17)
0.9	0.011795(39)	0.7527(1)	0.014435(48)	5.97235(16)
0.92	0.013783(67)	0.7427(1)	0.016686(81)	5.84091(21)
0.94	0.016237(79)	0.7328(1)	0.01952(10)	5.80088(26)
0.96	0.018686(63)	0.7224(1)	0.02228(07)	5.66382(30)
0.98	0.021625(75)	0.7120(1)	0.02567(09)	5.51804(44)
1	0.024843(87)	0.7009(1)	0.02938(10)	5.46904(50)
1.02	0.02823(10)	0.6899(1)	0.03329(12)	5.31864(67)
1.04	0.03216(11)	0.6785(1)	0.03795(13)	5.15826(69)
1.06	0.03623(09)	0.6664(1)	0.04277(11)	4.9978(11)
1.08	0.04058(10)	0.6537(2)	0.04799(11)	4.8332(12)

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T	p^s	ρ'	ρ''	Δh_v
1.1	0.04568(12)	0.6409(2)	0.05443(14)	4.7536(16)
1.12	0.05112(13)	0.6275(2)	0.06145(15)	4.5688(18)
1.14	0.05674(16)	0.6133(2)	0.06885(19)	4.3817(24)
1.16	0.06323(20)	0.5985(2)	0.07810(24)	4.1717(33)
1.18	0.06957(21)	0.5820(2)	0.08715(26)	3.9681(39)
1.2	0.07684(25)	0.5639(3)	0.09862(32)	3.7339(59)
1.22	0.08429(33)	0.5446(4)	0.11101(44)	3.3941(87)
1.24	0.09260(36)	0.5235(5)	0.12657(50)	3.122(11)
1.26	0.10129(44)	0.5007(5)	0.14451(62)	2.823(16)
1.28	0.11082(39)	0.4747(8)	0.17041(60)	2.350(21)

Table S4: Identified outliers in the best VLE data sets: *Errington*,[126,127] *Janeček et al.*,[135,136] *Lotfi et al.*,[71] *Mick et al.*,[23] *Okumura and Yonezawa*,[121,122] and this work.

Reference	T	p^s	ρ'	ρ''	Δh_v
Mick et al.[23]	0.75	0.0022(1)	0.8208(2)	0.0030(1)	6.595(3)
	1.25	0.0967(4)	0.514(2)	0.135(2)	3.30(3)
this work[(a)]	1.08	0.040583(62)	0.65371(20)	0.047992(74)	4.8332(12)
Lotfi et al.[71]	0.7	0.00131(6)	0.84266(18)	0.00193(10)	6.758(4)
Errington[125]	1.3	0.1212(10)	0.4271(13)	0.2096(13)	-
Errington[126,127]	1.3	0.1215841(996)	0.4442(51)	0.193072(5552)	-
	1.25	0.0975052(672)	0.5049(12)	0.143990(335)	-

[(a)] data point is slightly off the statistical uncertainties regarding the self-consistency Clausius-Clapeyron test (see Fig. S3).

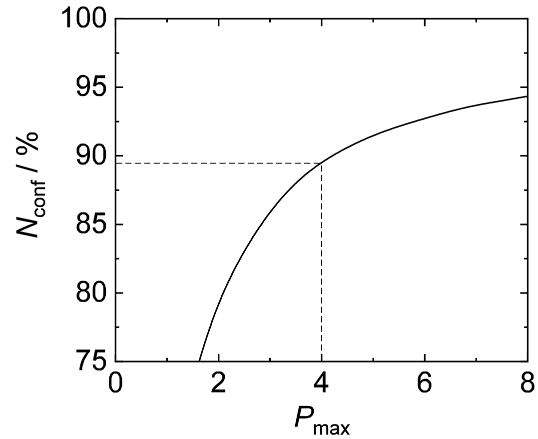

Figure S1: Percentage of overall confirmed data as a function of the parameter $P_{\max}$ for the homogeneous data EOS test. N_{conf} is the confirmation rate of all homogeneous data. The dashed line indicates the value $P_{\max} = 4$ chosen for the identification of outliers as they are specified in the database.

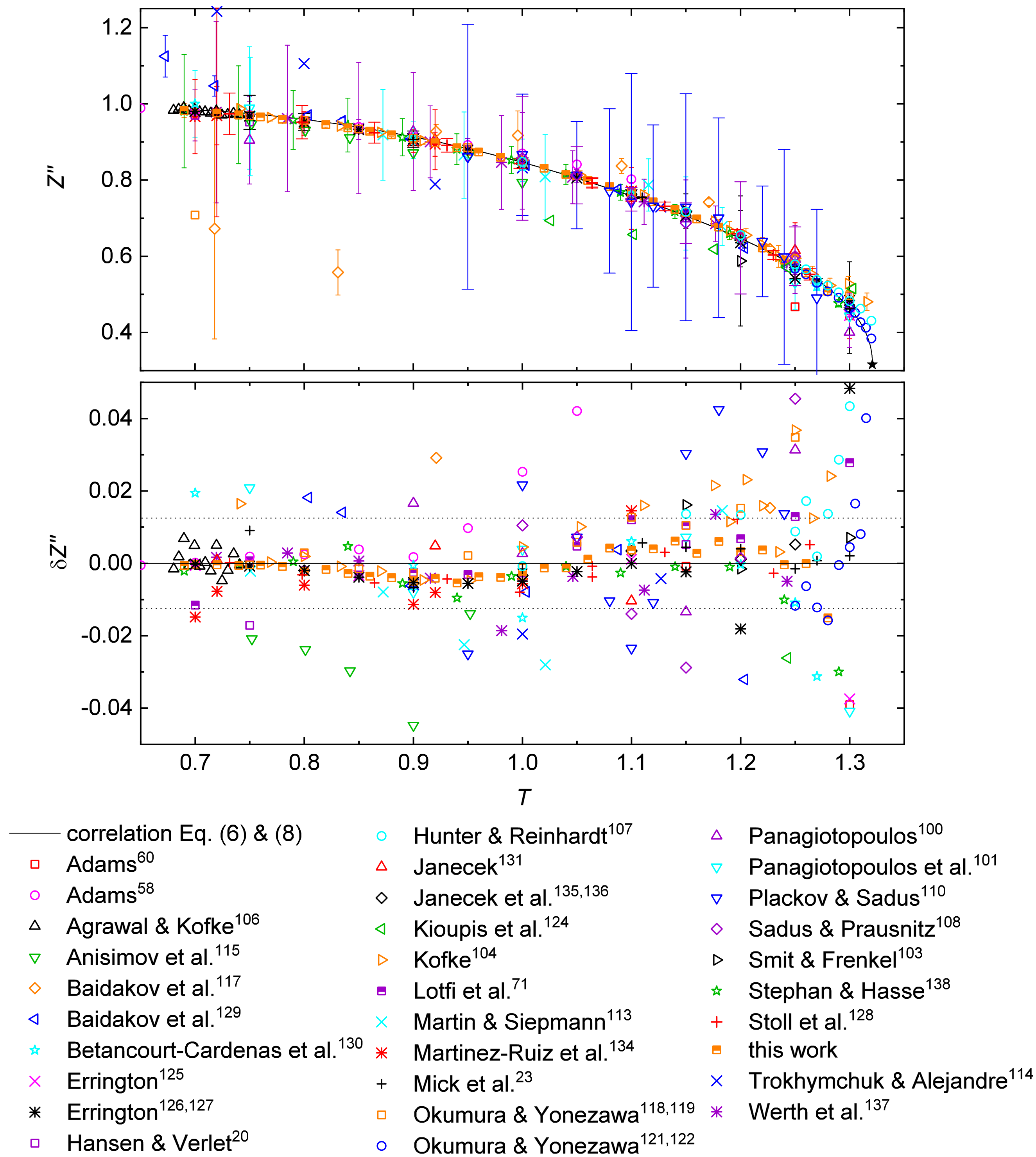

Figure S2: Compressibility factor test for the vapor-liquid equilibrium data of the Lennard-Jones fluid according to *Nezbeda*:[213,214] saturated vapor phase compressibility factor Z'' as function of the temperature T (top) and the relative deviation of Z'' from correlations (6) and (8) (bottom). The dotted line indicates the range of 2.5 times the confidence interval of the most precise data, as discussed in the main part of this work. Error bars are omitted in the bottom plot to avoid visual clutter. For clarity, the out-of-range data points are omitted in both, the top and bottom plot. The black filled star indicates the compressibility factor at the critical point according the base correlation.

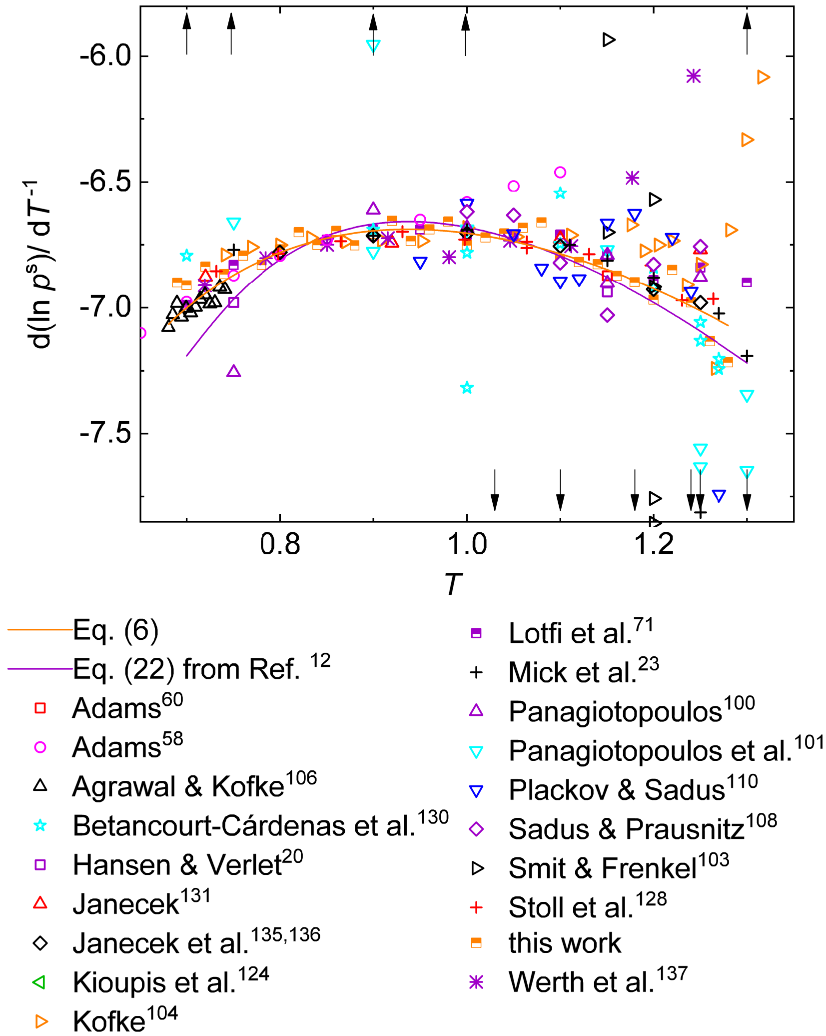

Figure S3: Clausius-Clapeyron test according to Eq. (10). Symbols indicate the RHS and the lines the LHS of Eq. (10). The orange line indicates Eq. (6). The purple line is Eq. (22) from Ref.[71] For clarity, the numeric values of the out-of-range data points are omitted in the plot; they lie in the range of $\mathrm{d}(\ln p^s)/\mathrm{d}(T^{-1}) = -31$ to -0.8.

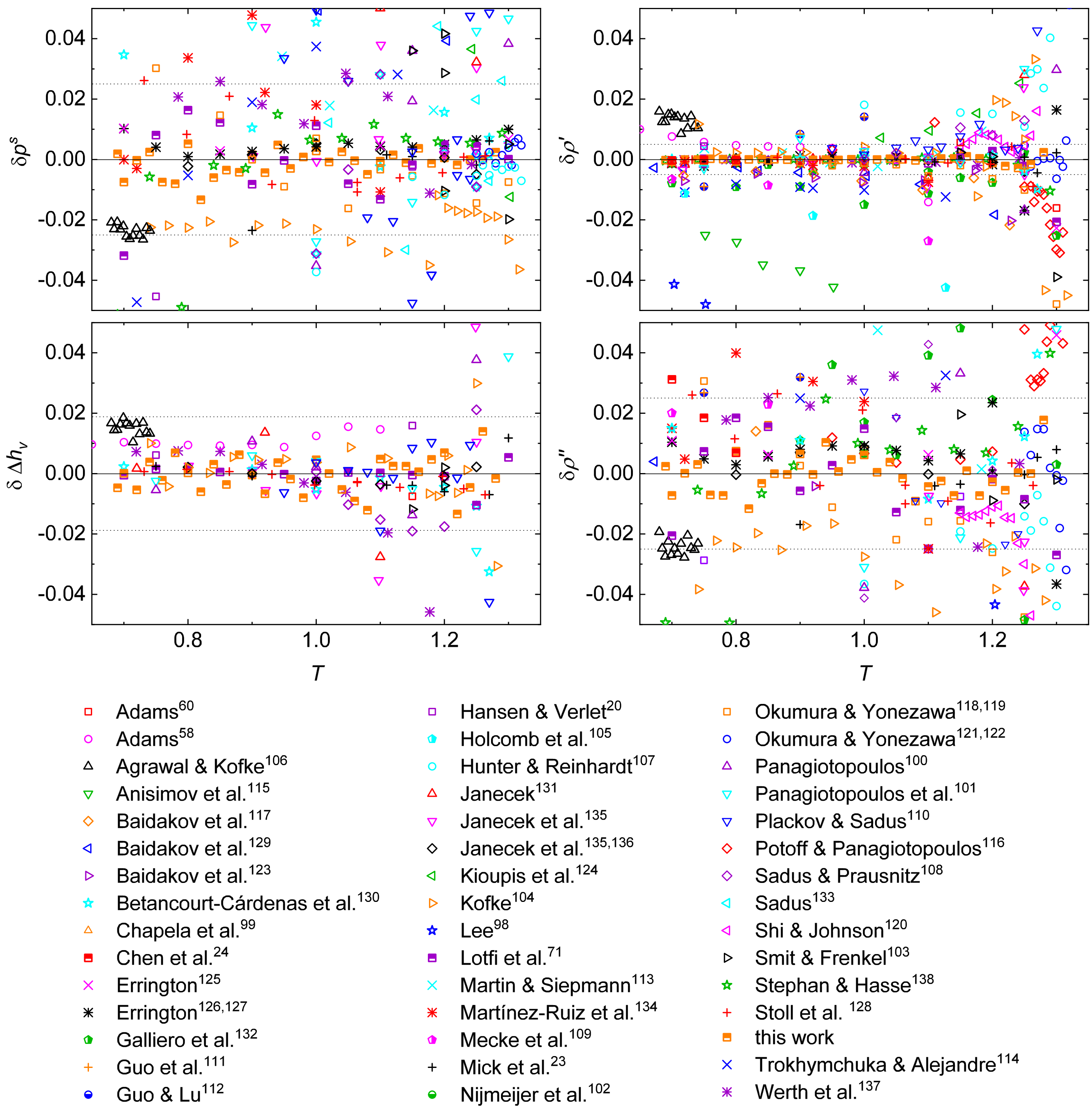

Figure S4: Relative deviations of the vapor-liquid equilibrium data for the vapor pressure p^s, saturated liquid density ρ', saturated vapor density ρ'', and enthalpy of vaporization Δh_v from correlations (6) - (9) as a function of the temperature T. Error bars were omitted to avoid visual clutter. The dotted lines indicates the range of 2.5 times the confidence interval of the most precise data δx, as discussed in the main part of this work. Error bars are omitted in the plots to avoid visual clutter. For clarity, the out-of-range data points are omitted in the deviation plots.

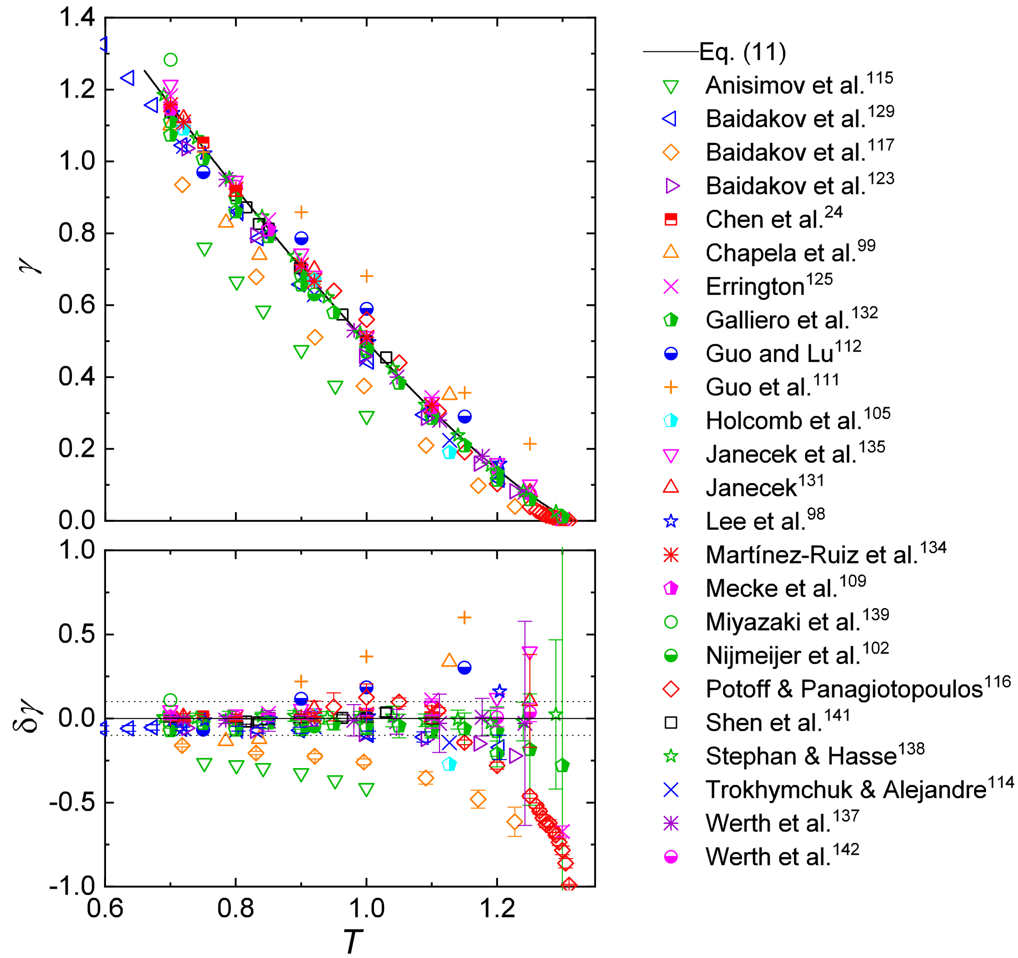

Figure S5: Surface tension of the LJ fluid as a function of the temperature (top) and the corresponding relative deviation plot (bottom). The black line indicates Eq. (11). Symbols indicate computer experiment data. For clarity, numerical values for out-of-range data points in the vicinity of the critical temperature in the deviation plot are omitted. The dotted lines indicates the range of 2.5 times the confidence interval of the most precise data as discussed in the main part of this work.