Thermodynamic Properties of HFE-7300

Supporting information

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1. Testing of the critical point experiments

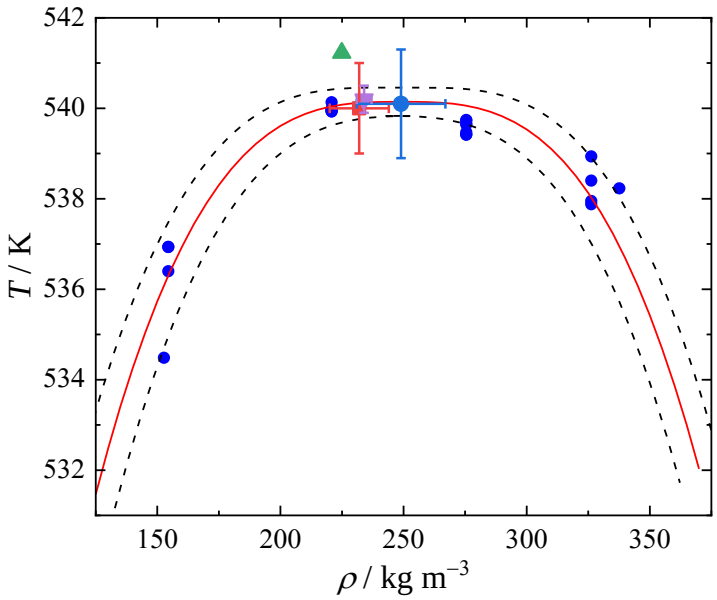

Figure S1. Determination of critical temperature and density of *n*-heptane by DSC and comparison to reference values.
●, observed T_{step} temperatures; ━, two-phase envelope description with critical scaling law, Equation (1) in the main text; ╍, statistic part of standard uncertainty of the description u_A; ●, evaluated ρ_C and T_C with expanded uncertainty (k = 2) error bars. ■, ρ_C and T_C obtained using the DSC method by Steele (private communication cited in [1]). ▼, Critically evaluated reference ρ_C and T_C [1]. ▲, ρ_C and T_C used in the multiparameter equation of state [2] implemented in REFPROP [3].

2. Testing of the ebulliometric method

Table S1
Vapor pressures of reference compounds determined within testing of the ebulliometer

Demineralized water (liquid)			Toluene (liquid)			Acetone (liquid)		
T / K	p_{sat} / Pa	$p_{sat}-p_{ref}$ / Pa	T / K	p_{sat} / Pa	$p_{sat}-p_{ref}$ / Pa	T / K	p_{sat} / Pa	$p_{sat}-p_{ref}$ / Pa
372.743	99992	38	372.733	73327	16	328.810	99992	68
370.824	93326	42	372.722	73327	41	328.034	97325	30
368.789	86660	41	369.685	66661	−102	323.606	83326	−6
366.626	79993	21	367.627	62662	50	319.297	71327	−3
364.284	73327	67	365.548	58662	33	314.857	60395	−62
361.771	66661	75	363.335	54662	48	310.369	50796	−69
359.043	59995	71	360.986	50663	66	305.972	42663	−37
354.743	50663	104	358.534	46663	5	301.499	35464	−57
372.739	99992	52	355.822	42663	70	297.050	29331	−57
368.143	84660	73	352.952	38663	57	292.522	23998	−67
363.299	70661	80	349.825	34664	53	287.937	19465	−44
358.170	57995	82	372.738	73327	5			
353.064	47329	79	369.633	66661	6			
348.132	38663	96	367.665	62662	−25			
343.094	31331	204	383.276	99992	14			
338.365	25331	47	380.877	93326	−4			
372.376	98659	10	378.341	86660	−22			
368.153	84660	41	375.639	79993	−25			
363.319	70661	27						
358.186	57995	45						
353.083	47329	42						
348.165	38663	43						
343.233	31331	16						
338.425	25331	−21						
333.198	19998	7						
328.115	15732	−4						
323.262	12399	−22						
318.380	9599	−110						

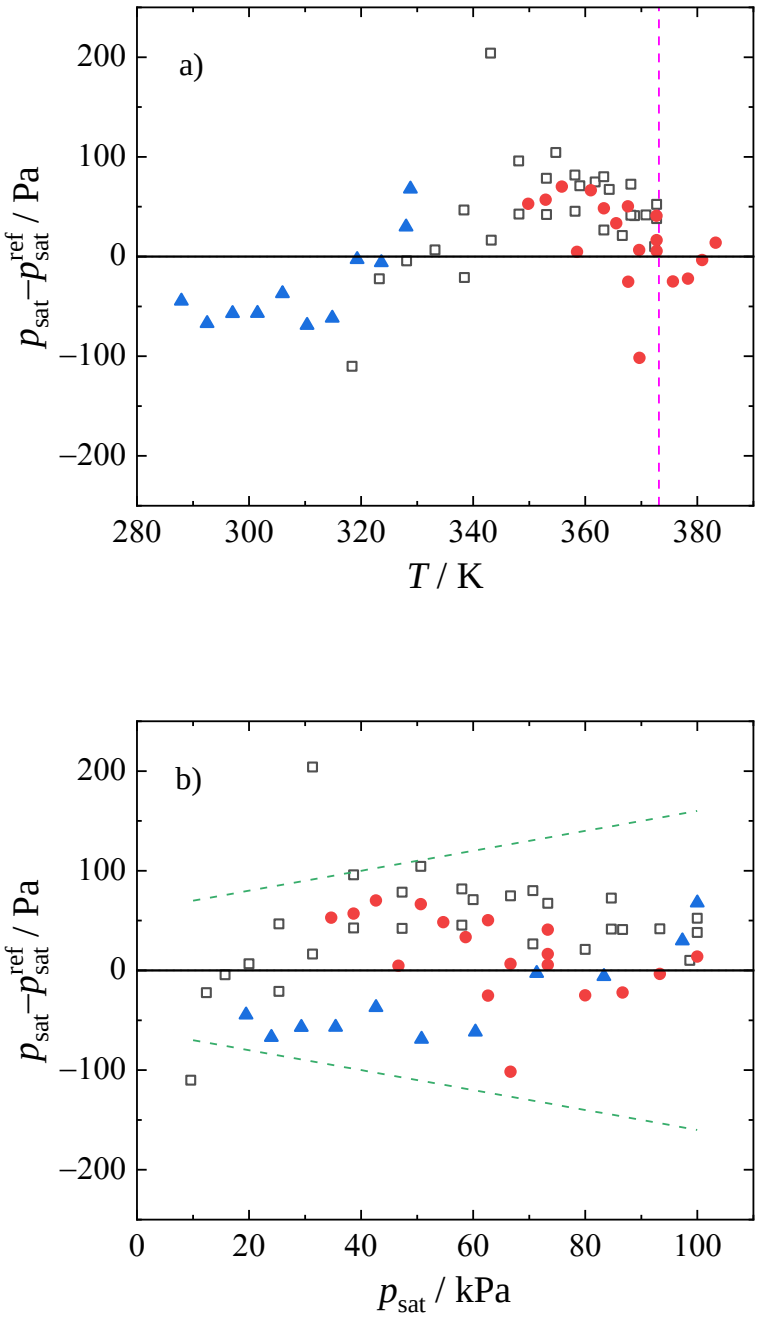

Figure S2. Comparison of vapor pressures of reference compounds used for testing of the ebulliometer to the reference values as a function of a) temperature and b) pressure.
●, Toluene (reference: [4]); □, demineralized water (reference: [5]); ▲, acetone (reference: [6]); **--**, upper limit of the thermistor calibration; **--**, combined expanded uncertainty of $U_c\left(p_{sat}/\mathrm{Pa}\right)=0.001\left(p_{sat}/\mathrm{Pa}\right)+60$ proposed for HFE-7300, see Section 3.5 for details.

3. Ideal-gas thermodynamic properties

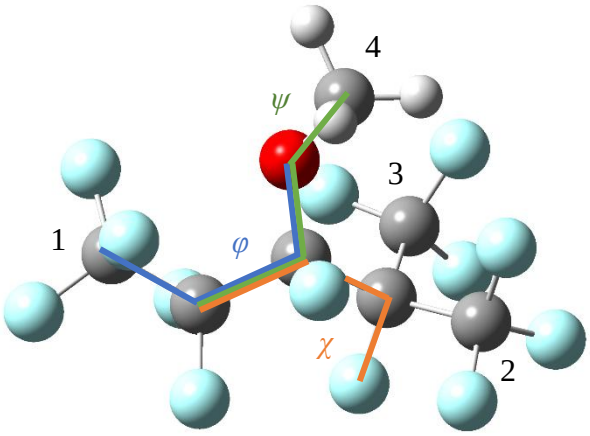

Figure S3. Most stable conformer of (*S*)-HFE-7300 at the B3LYP-D3/6-311+G(2df,p) level of theory. The conformer-defining angles are depicted: Blue: φ, orange: χ, green: ψ. Numbers label rotating tops.

Table S2
Stable conformers of (*S*)-HFE-7300 and their characteristics. [a]

#	Conformer [b]	φ [b] / °	χ [b] / °	ψ [b] / °	$\Delta_r E_i^{0\,K}$	$\Delta_r H_i^{0\,K}$	μ / D	$I_A I_B I_C \cdot 10^{135}$ / kg^{3}m^6	Ex. Freq. [c]
36	n'n'o	−44.1	−20.9	148.1	0	0	2.75	18562	2,4,5,7
38	e'g'g	−109.9	−46.7	71.9	0.845	0.840	2.79	18642	3,4,5,7
39	g'n'e	−46.5	−26.2	109.4	1.826	0.864	2.75	18527	1,4,5,8
35	gn'g	58.1	−20.1	63.1	2.261	2.255	2.78	16736	3,4,5,11
20	tn'g	161.7	−44.6	60.9	2.854	6.877	2.94	18755	2,3,5,11
23	tg'g	−178.2	−65.7	69.6	3.179	2.928	2.72	17095	1,2,3,11
22	g'g'e	−68.3	−69.3	108.9	3.925	3.358	2.72	18359	3,4,6,7
33	g'tt	−79.3	−173.7	161.1	4.230	4.200	2.51	17759	3,4,5,8
8	g'to	−45.2	−162.2	155.2	4.452	4.278	2.49	17876	2,3,5,7
3	d'ng	−105.0	41.7	69.5	5.204	5.428	2.75	18079	2,4,5,11
1	nnd	32.9	29.9	80.5	5.296	5.139	2.69	17671	2,4,5,9
19	d'g'g	−92.5	−63.7	64.7	7.200	2.562	2.74	17139	2,3,4,12
24	ggg	49.7	78.8	72.3	7.853	7.724	2.58	16958	1,3,6,7
28	g'ge	−51.6	74.8	106.1	7.938	7.622	2.63	18423	3,4,5,7
26	g'ne	−71.0	23.3	119.9	7.991	7.379	2.72	18835	2,3,5,6
32	d'tg	−104.5	−171.2	69.4	9.177	9.342	2.71	17224	2,4,5,11
13	g'oo	−73.0	159.1	138.6	9.967	8.764	2.47	17955	2,3,5,7
7	tng	178.2	23.2	70.6	11.211	10.977	2.68	17250	3,4,5,10
17	ng'g	30.5	−64.1	78.8	11.456	11.319	2.69	16797	1,3,5,10
5	tnd	−178.2	21.5	96.8	12.544	11.708	2.61	17185	3,5,6,7
11	e'tg	−110.9	167.9	72.5	12.978	12.927	2.65	17027	2,3,4,6
27	n'gg'	−40.0	71.2	−75.3	13.726	13.701	2.36	18069	2,4,5,11
9	go'o	58.9	−158.2	147.2	16.668	16.794	2.49	15732	1,4,5,7
10	go'g	53.6	−156.4	64.5	17.604	17.647	2.55	15680	1,4,5,12
37	g'g'g'	−54.7	−72.6	−55.5	17.706	18.092	2.65	17979	2,3,4,12
40	g'dt	−54.1	93.5	164.5	18.494	18.226	2.70	18990	2,3,5,16

#	Conformer [b]	φ [b] / °	χ [b] / °	ψ [b] / °	$\Delta_r E_i^{0\,K}$	$\Delta_r H_i^{0\,K}$	μ / D	$I_A I_B I_C \cdot 10^{135}$ / kg^{3}m^6	Ex. Freq. [c]
4	g'nn'	−66.5	33.0	−44.5	20.731	21.140	2.54	18662	3,4,5,9
31	gtt	64.0	−164.0	166.2	22.061	22.015	2.48	15215	1,3,4,10
14	toe	−174.0	159.5	129.3	23.654	22.778	2.35	16059	1,4,6,8
12	g'og'	−49.7	152.6	−69.0	25.353	25.354	2.47	17721	2,3,5,11
16	ttg	−176.4	161.7	77.2	25.412	24.765	2.43	16118	1,4,6,11
25	dgg'	93.4	51.9	−57.7	26.370	27.214	2.39	16312	1,3,4,13
6	tnn'	−169.5	24.6	−35.6	27.586	28.005	2.45	16846	2,4,5,11
30	tte	−178.7	174.3	128.1	27.638	26.751	2.32	15925	2,3,5,8
21	g'n'n'	−70.9	−39.3	−31.2	27.820	27.522	2.78	18831	2,4,5,12
15	o'og'	−157.3	151.5	−65.5	40.612	40.421	2.41	15771	1,2,4,12
34	ton'	−167.3	159.4	−25.7	42.845	42.303	2.51	15692	2,3,6,11
29	teo	−164.7	110.1	153.6	46.986	46.821	2.33	16882	1,4,5,12
2	nng'	41.1	39.3	−72.8	48.000	48.557	2.70	17992	3,4,5,11
18	gg'd'	45.5	−63.8	−82.5	48.370	49.011	2.83	16555	1,3,5,11

[a] $\Delta_r E^{0\,K}$ and $\Delta_r H^{0\,K} = \Delta_r E^{0\,K} + \Delta_r E^{ZPE}$ is the relative electronic energy and enthalpy, respectively, in kJ mol^{-1} with respect to the most stable conformer. $\Delta_r E^{ZPE}$ is the zero-point vibrational energy. μ is the dipole moment in Debyes. $I_A I_B I_C$ is the product of principal moments of inertia.

[b] Used dihedral angle labels: c ≈ 0°, n ≈ 30°, g ≈ 60°, d ≈ 90°, e ≈ 120°, o ≈ 150°, and t ≈ 180°. Primes denote negative dihedral angles. Consult Figure S3 for the meaning of characteristic dihedral angles φ, χ, and ψ.

[c] Numbers of vibrational modes assigned to internal rotations of terminal groups, which were excluded from the RRHO treatment.

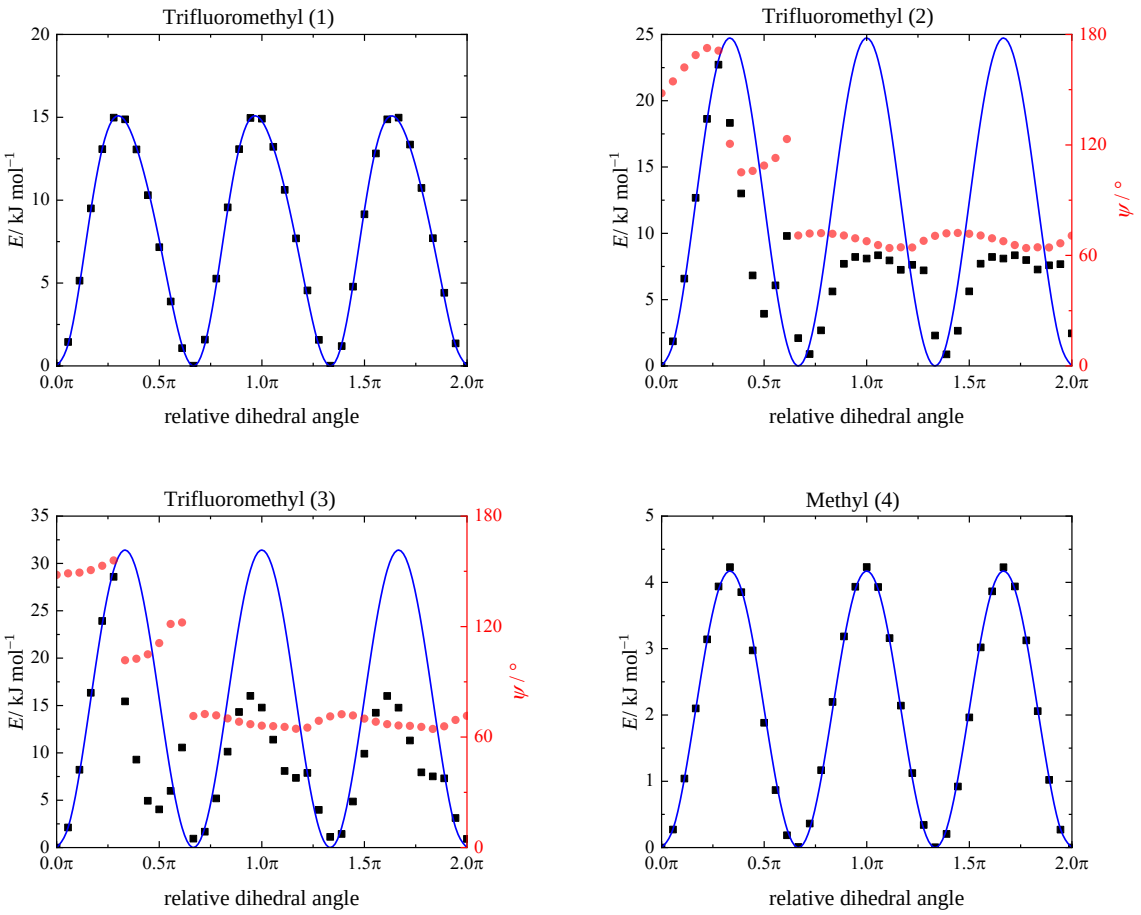

Figure S4. Potential energy profiles of the rotating tops.
■, Values calculated at the B3LYP-D3/6-311+G(2df,p) level of theory, —, representation by Fourier expansion (parameters in Table S3), ●, Values of dihedral angle ψ (position of methoxy top, right axis). For tops 2 and 3, the discontinuities correspond to transition to domain of another conformer through distortion of the dihedral angle ψ. Only the first few potential energy values corresponding to the original conformer were described by the Fourier expansion for these tops.

Table S3
Reduced moments of inertia I_r, internal symmetry number σ_I, and Fourier expansion parameters of methyl rotations used in the R1SM approach.

Top [a]	I_r [b] / 10^{-47} kg m^2	σ_I	Fourier expansion parameters [c] / J mol^{-1}
Trifluoromethyl (1)	137.37 ± 1.76	3	$V_0 = 7943$, $V_3^{cos} = -7390$, $V_3^{sin} = 929$, $V_6^{cos} = -552$, $V_6^{sin} = -478$
Trifluoromethyl (2)	138.69 ± 1.49	3	$V_0 = 12364$, $V_3^{cos} = -12364$
Trifluoromethyl (3)	138.76 ± 1.46	3	$V_0 = 15709$, $V_3^{cos} = -15709$
Methyl (4)	5.301 ± 0.014	3	$V_0 = 2086$, $V_3^{cos} = -2086$

[a] Consult Figure S3 for the meaning of top labels.

[b] Mean reduced moment of inertia of the given top in all conformers and standard deviation of the mean.

[c] Fourier expansion has the form: $V(\varphi) = V_0 + \sum_i V_i^{cos} \cos(i\varphi) + V_i^{cos} \sin(i\varphi)$. The parameters not listed were found redundant and were set to zero. Rotational profiles calculated for the most stable conformer were always used for all conformers.

4. Critical properties

Table S4
Masses *m*, loading densities ρ, and temperatures of the step change of DSC signal T_{step} observed during measurements of critical temperature and density.

Experiment	m / mg	ρ / kg m^{-3} ∘	T_{step} / K	$\Delta\rho$ / kg m^{-3} ∘	ΔT_{step} / K
CH323.2	17.99	445.3	505.00	−24.76	0.94
CH323.4	17.95	444.3	505.50	−42.56	1.48
	17.95	444.3	505.56	−44.83	1.54
	17.95	444.3	505.54	−44.22	1.53
CH324.1	21.42	530.2	505.82	30.34	−0.55
	21.42	530.2	505.69	35.73	−0.68
	21.42	530.2	505.72	34.48	−0.65
CH324.2	21.42	530.2	505.38	47.59	−0.99
	21.42	530.2	505.39	47.16	−0.98
	21.42	530.2	505.43	45.94	−0.94
CH329.1	31.54	780.7	505.61	−15.87	−0.36
	31.54	780.7	505.71	−12.02	−0.27
	31.54	780.7	505.68	−12.93	−0.29
CH330.1	30.95	766.1	505.36	−39.65	−0.88
	30.95	766.1	505.26	−43.33	−0.99
	30.95	766.1	505.53	−33.49	−0.71
CH330.2	30.95	766.1	506.61	29.05	0.37
	30.95	766.1	506.53	21.24	0.29
	30.95	766.1	506.71	40.86	0.47
CH332.1	27.06	669.8	506.12	– [a]	−0.78
	27.06	669.8	506.38	– [a]	−0.52
	27.06	669.8	506.51	– [a]	−0.39
CH332.2	27.02	668.8	506.01	– [a]	−0.89
	27.02	668.8	505.56	– [a]	−1.35
	27.02	668.8	505.59	– [a]	−1.32
	27.02	668.8	505.54	– [a]	−1.36
CH336.1	24.15	597.8	507.91	– [a]	1.04
	24.15	597.8	507.42	– [a]	0.55
	24.15	597.8	507.72	– [a]	0.85
	24.15	597.8	507.71	– [a]	0.83
CH337.1	24.25	600.2	506.48	– [a]	−0.39
	24.25	600.2	506.34	– [a]	−0.54
CH337.2	23.97	593.3	507.24	– [a]	0.38
	23.97	593.3	506.27	– [a]	−0.59
	23.97	593.3	507.13	– [a]	0.27
CH346.1	38.84	961.4	497.35	20.21	2.08
CH346.2	38.84	961.4	497.42	20.98	2.16
CH350.1	17.57	434.9	504.54	−22.30	0.95
	17.57	434.9	504.69	−26.15	1.10
	17.57	434.9	504.43	−19.33	0.84
CH350.2	17.57	434.9	504.46	−20.03	0.87
	17.57	434.9	504.61	−23.98	1.02
CH362.1	14.67	363.1	501.27	−31.31	2.40

Experiment	m / mg	ρ / kg m^{-3}∘	T_{step} / K	$\Delta\rho$ / kg m^{-3}∘	ΔT_{step} / K
	14.67	363.1	501.61	−36.52	2.75
CH362.2	14.58	360.9	501.40	−35.52	2.73
	14.58	360.9	501.52	−37.32	2.85
	14.58	360.9	501.61	−38.66	2.94
CH362.5	14.58	360.9	502.19	−48.07	3.53
	14.58	360.9	502.42	−51.86	3.75
	14.58	360.9	502.67	−56.32	4.01
CH364.1	34.98	865.8	502.76	−3.09	−0.17
	34.98	865.8	502.83	−1.83	−0.10
	34.98	865.8	503.17	4.65	0.24
CH332.3	27.02	668.8	505.15	– [a]	−1.75
	27.02	668.8	505.34	– [a]	−1.57
	27.02	668.8	505.27	– [a]	−1.64
	27.02	668.8	505.08	– [a]	−1.82
CH324.5	21.42	530.2	505.47	44.59	−0.91
	21.42	530.2	505.44	45.69	−0.94
	21.42	530.2	505.40	47.13	−0.98
CH324.7	21.42	530.2	505.32	49.92	−1.06
	21.42	530.2	505.38	47.83	−1.00
	21.42	530.2	505.33	49.58	−1.05
CH343.2	10.74	265.8	483.71	21.61	−3.56
	10.74	265.8	484.03	19.75	−3.24
	10.74	265.8	484.38	17.71	−2.89
CH343.4	10.74	265.8	484.20	18.76	−3.07
	10.74	265.8	484.72	15.70	−2.55
	10.74	265.8	484.75	15.52	−2.52
CH365.2	12.12	300.0	494.21	−17.02	2.09
	12.12	300.0	493.94	−14.71	1.82
	12.12	300.0	493.57	−11.60	1.45
CH365.3	12.03	297.8	491.84	0.01	0.00
	12.03	297.8	491.38	3.44	−0.45
	12.03	297.8	491.10	5.53	−0.73
σ [b]				28	1.6

[a] $\Delta\rho$ cannot be evaluated for points in the critical loci.

[b] Root mean square deviation, $\sigma(X) = \left(\frac{1}{n} \sum_{i=1}^{n} \Delta X_i^{\,2} \right)^{1/2}$.

5. Vapor pressure correlation

Table S5

Tabulated vapor pressures and vaporization thermodynamic functions of liquid HFE-7300

T/K	p / Pa	U_c [a]/ Pa	ψ [b]/ kJ mol^{-1}	U_c / kJ mol^{-1}	$\Delta_l^g H_m$ / kJ mol^{-1}	U_c / kJ mol^{-1}	$\Delta C'$ / J K^{-1} mol^{-1}	U_c / J K^{-1} mol^{-1}	$\Delta_l^g C_{p,m}^0$ / J K^{-1} mol^{-1}	U_c / J K^{-1} mol^{-1}
215	7.592	0.081	45.42	0.40	45.41	0.40	−91.8	12.5	−92.0	12.6
220	13.49	0.12	44.96	0.34	44.95	0.34	−90.7	11.5	−91.0	11.6
230	38.85	0.22	44.06	0.25	44.05	0.25	−88.3	9.4	−88.8	9.7
240	100.53	0.41	43.19	0.18	43.17	0.19	−85.7	7.6	−86.7	8.0
250	236.97	0.75	42.35	0.14	42.31	0.16	−83.0	5.8	−84.6	6.7
260	514.90	1.40	41.53	0.11	41.47	0.14	−80.2	4.4	−82.6	5.6
270	1042.0	2.4	40.75	0.10	40.64	0.15	−77.3	3.3	−80.8	5.1
273.15	1283.9	2.9	40.51	0.10	40.38	0.16	−76.3	3.0	−80.2	5.0
280	1980.7	4.4	39.99	0.09	39.82	0.17	−74.2	2.6	−79.1	5.1
290	3562.2	7.7	39.26	0.08	39.02	0.20	−71.0	2.5	−77.6	5.8
298.15	5542	12	38.70	0.07	38.36	0.23	−68.4	2.7	−76.5	6.7
300	6101	13	38.57	0.07	38.21	0.24	−67.8	2.8	−76.2	7.0
310	10003	21	37.91	0.06	37.41	0.31	−64.4	3.1	−74.9	8.4
320	15780	31	37.28	0.07	36.61	0.40	−61.0	3.5	−73.7	9.8
330	24046	42	36.69	0.08	35.8	0.5	−57.4	3.7	−72.4	11.1
340	35525	52	36.13	0.11	35.0	0.7	−53.7	3.7	−71.0	12.1
350	51051	65	35.62	0.14	34.2	0.8	−49.8	3.6	−69.4	13.0
360	71556	98	35.14	0.17	33.4	1.0	−45.8	3.3	−67.6	13.7
370	98080	180	34.70	0.19	32.6	1.2	−41.7	2.8	−65.4	14.1
370.64	100010	190	34.67	0.20	32.5	1.3	−41.4	2.8	−65.3	14.1
380	131750	330	34.30	0.22	31.8	1.5	−37.3	2.2	−62.9	14.4
390	173790	580	33.96	0.23	31.0	1.7	−32.7	1.5	−60.0	14.8
400	225530	930	33.65	0.23	30.2	1.9	−27.8	1.1	−56.8	16.0
410	288400	1400	33.40	0.23			−22.5	1.8		
420	363900	2100	33.20	0.20			−17.0	3.2		
430	453700	3100	33.06	0.17			−10.9	4.9		
440	559700	4500	32.99	0.11			−4.3	7.0		
450	683800	6500	32.98	0.05			3.1	9.4		
460	828400	9500	33.05	0.10			11.6	12.4		
470	996000	14000	33.22	0.23			21.7	16.1		
480	1190000	21000	33.50	0.41			34.6	21.2		
490	1414000	35000	33.9	0.7			53.8	29.5		
500	1672000	59000	34.6	1.0			96.7	49.6		
506.9	1876000	94000	36.0	1.7			∞	−		

[a] Expanded uncertainties of the corresponding properties developed though the Monte Carlo method and error propagation law.

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

6. Equations of state

Table S6

Summary of used data sets for the fitting procedure

Property	Reference	Year	Number of exp. points	Temperature range T / K	Pressure range p / kPa	Relative expanded uncertainty (k = 2) $100U_r$
p^{sat}	This work, UCT, Ebulliometry	2025	37[a]	310.0 – 369.8	10.0 – 97.3	≤ 0.7
	This work, UCT, STAT6	2025	48[a]	233.3 – 308.0	0.05 – 9.09	≤ 0.6
pVT	This work, IT CAS	2025	85[a]	263.3 – 423.8	100.4 – 59990	< 0.15
	This work, TUC	2025	35	263.5 – 422.1	115.5 – 90200	< 0.12
	Prokopová et al. [7]	2023	30[a]	273.2 – 343.2	98.2	< 0.01
	Vinš et al. [8]	2021	25	264.5 – 343.4	98.0	< 0.04
	Muñoz-Rujas et al. [9]	2018	96	293.2 – 393.2	100 – 60000	< 0.05
	Rausch et al. [10]	2015	19	273.2 – 363.2	1.91 – 85.5	0.02
C_p	This work, UCT, Microcalvet	2025	41[a]	245.0 – 350.0	100	0.6
	This work, UCT, PE 8500	2025	31	215.8 – 365.2	100	2.0
c	This work, TUC	2025	34	262.3 – 424.4	122 – 90170	< 0.02
	Muñoz-Rujas et al. [9]	2018	6	293.2 – 529.0	100 – 48.1	< 0.2

[a] Values from multiple measurements at similar conditions were averaged in the fitting routine.

Table S7

Complete set of fitted parameters for various EOS and AARD for **overall optimization**. For EOS with subscript LCP (loose critical point), the critical properties can be parameters in the fitting procedure that lie outside the experimental uncertainties for the critical properties

EOS	parameter of EOS							100 AARD				
[a]	T_C / K	p_C / MPa	ω / -					Over-all	ρ	p^{sat}	C_p	c
LKP	508.09	1.785	0.4267					3.17	1.44	7.32	2.77	12.02
LKP_{LCP}	524.38	1.824	0.4300					2.55	0.78	6.18	2.71	11.65
LKP-SJT1	505.71	1.864	0.4344					7.01	6.76	9.76	2.54	10.16
$LKP\text{-}SJT1_{LCP}$	503.84	2.548	0.4352					6.98	6.77	9.38	2.51	10.12
LKP-SJT2	505.38	1.890	0.4346					6.24	5.80	9.06	2.49	10.03
$LKP\text{-}SJT2_{LCP}$	528.24	1.535	0.4349					6.23	5.80	8.95	2.48	10.02
PR	505.06	1.811	0.5110					3.16	1.32	2.94	3.76	15.12
PR_{LCP}	500.89	1.794	0.5307					3.04	1.23	2.40	3.31	15.36
PR*	513.32	1.863	0.4351					4.79	2.05	14.46	5.74	15.28
SRK	505.17	1.969	0.5250					4.11	2.52	4.99	2.26	15.53
SRK_{LCP}	514.40	2.074	0.4635					3.08	1.41	1.48	3.52	15.01
[b]				L / -	M / -	N / -	c / cm^3 mol^{-1}					
PR-TWU-C	508.09	1.812	0.4885	2.29374	1.65794	0.31169	1.1777	2.81	1.28	0.79	1.63	15.44
$PR\text{-}TWU\text{-}C_{LCP}$	507.45	1.808	0.5249	0.78987	0.76586	1.17753	1.1777	3.05	1.25	3.33	2.41	15.36
[c]				C_1 / -	C_2 / -	C_3 / -						
SRK-MC	505.17	1.969	0.5699	1.37999	−0.91447	1.53785		3.80	2.54	2.20	1.00	15.54
$SRK\text{-}MC_{LCP}$	520.91	2.113	0.6377	1.12229	−0.35994	0.95068		3.71	1.73	9.03	0.90	15.25
[d]	m / -	σ / Å	ε/k_b / K	n_μ / -	μ / D							
PCP-SAFT	4.91975	3.75837	192.903	1	2.4361			3.20	1.35	0.77	0.47	19.42
PCP-SAFT**	4.94245	3.74834	192.542	1	2.4549			3.24	1.48	0.13	0.42	19.39

[a] Critical temperature T_C, critical pressure p_C, acentric factor ω. Star denotes parameters developed by Aminian et al. [11].

[b] L, M and N parameters for the modified SRK and volume correction c.

[c] C_1, C_2, and C_3 parameters of the Mathias-Copeman α-function.

[d] Segment number m, segment diameter σ, energy parameter ε/k_b, number of dipoles n_μ, and dipole moment μ. Double star denotes parameters developed by Vinš et al. [8].

Table S8
Complete set of fitted parameters for various EOS and AARD for **density optimization**. For EOS with subscript LCP (loose critical point), the critical properties can be parameters in the fitting procedure that lie outside the experimental uncertainties for the critical properties.

EOS	parameter of EOS							100 AARD				
[a]	T_C / K	p_C /MPa	ω / -					Over-all	ρ	p^{sat}	C_p	c
LKP	508.80	1.782	0.4187					3.07	0.75	11.44	2.92	12.59
LKP_{LCP}	488.21	1.638	0.4724					3.86	0.53	29.88	3.34	7.58
LKP-SJT1	507.36	1.795	0.3500					10.70	5.13	62.23	5.08	14.85
$LKP\text{-}SJT1_{LCP}$	517.25	1.687	0.3500					10.70	5.13	62.23	5.08	14.85
LKP-SJT2	507.36	1.827	0.3500					9.91	4.18	61.21	5.03	14.74
$LKP\text{-}SJT2_{LCP}$	496.33	2.436	0.3500					9.91	4.18	61.21	5.03	14.74
PR	505.00	1.791	0.6223					5.63	1.23	39.42	1.89	13.43
PR_{LCP}	484.28	1.741	0.6500					3.48	1.17	9.41	1.98	15.72
PR*	513.32	1.863	0.4351					4.79	2.05	14.46	5.74	15.28
SRK	505.00	1.970	0.6500					6.35	1.80	42.89	2.05	13.51
SRK_{LCP}	500.11	2.001	0.6500					5.01	1.13	31.65	2.09	13.84
[b]				L / -	M / -	N / -	c / cm^3 mol^{-1}					
PR-TWU-C	505.86	1.811	0.4926	0.38728	0.52386	1.57616	−2.7635	7.96	1.02	52.87	19.27	12.96
$PR\text{-}TWU\text{-}C_{LCP}$	490.62	1.799	0.5330	1.66754	0.23149	0.96266	−6.6549	7.24	0.88	41.74	21.33	13.75
[c]				C_1 / -	C_2 / -	C_3 / -						
SRK-MC	505.00	1.970	0.6242	1.31688	1.78052	1.99723		10.56	0.78	77.70	29.11	12.79
$SRK\text{-}MC_{LCP}$	496.52	1.949	0.6271	1.41375	1.52735	1.59953		9.63	0.75	71.38	24.81	12.32
[d]	m / -	σ / Å	ε/k_b / K	n_μ / -	μ / D							
PCP-SAFT	5.00000	3.76110	200.000	1	2.8000			6.45	1.01	51.50	0.50	14.71
PCP-SAFT**	4.94245	3.74834	192.542	1	2.4549			3.24	1.48	0.13	0.42	19.39

[a] Critical temperature T_C, critical pressure p_C, acentric factor ω. Star denotes parameters developed by Aminian et al. [11].

[b] L, M and N parameters for the modified SRK and volume correction c.

[c] C_1, C_2, and C_3 parameters of the Mathias-Copeman α-function.

[d] Segment number m, segment diameter σ, energy parameter ε/k_b, number of dipoles n_μ, and dipole moment μ. Double star denotes parameters developed by Vinš et al. [8].

Table S9

Complete set of fitted parameters for various EOS and AARD for **vapor pressure optimization**. For EOS with subscript LCP (loose critical point), the critical properties can be parameters in the fitting procedure that lie outside the experimental uncertainties for the critical properties.

EOS	parameter of EOS							100 AARD				
[a]	T_C / K	p_C / MPa	ω / -					Over-all	ρ	p^{sat}	C_p	c
LKP	505.00	1.970	0.4456					11.66	13.75	1.96	2.65	11.76
LKP_{LCP}	492.36	2.015	0.4526					15.90	19.75	0.35	2.71	11.70
LKP-SJT1	507.26	1.867	0.4485					6.68	7.02	4.81	2.05	9.34
$LKP\text{-}SJT1_{LCP}$	510.88	2.237	0.4485					6.68	7.02	4.81	2.05	9.34
LKP-SJT2	508.75	1.829	0.4466					5.98	6.02	5.15	2.14	9.33
$LKP\text{-}SJT2_{LCP}$	532.25	1.740	0.4466					5.98	6.02	5.15	2.14	9.33
PR	505.00	1.922	0.5232					7.00	6.97	1.14	3.55	14.09
PR_{LCP}	483.18	1.317	0.5998					19.62	7.87	0.27	2.30	12.04
PR*	513.32	1.863	0.4351					4.79	2.05	14.46	5.74	15.28
SRK	506.06	1.854	0.4961					8.10	8.20	0.81	2.79	16.80
SRK_{LCP}	491.70	1.454	0.5454					21.34	25.71	0.45	1.95	22.31
[b]				L / -	M / -	N / -	c / cm^3 mol^{-1}					
PR-TWU-C	508.33	1.823	0.5763	2.29923	1.65172	0.31169	−11.7449	5.10	4.53	0.16	1.53	15.25
$PR\text{-}TWU\text{-}C_{LCP}$	521.53	2.158	0.4243	2.08465	1.23102	0.38368	−14.2022	7.12	7.87	0.27	0.67	12.04
[c]				C_1 / -	C_2 / -	C_3 / -						
SRK-MC	506.40	1.837	0.5784	1.22007	−0.14838	0.42976		8.59	9.10	0.29	1.08	17.01
$SRK\text{-}MC_{LCP}$	521.03	2.378	0.5320	1.20703	−0.44441	0.88691		12.03	14.28	0.48	1.45	13.61
[d]	m / -	σ / Å	ε/k_b / K	n_μ / -	μ / D							
PCP-SAFT	4.99841	3.76865	191.054	1	2.4934			3.44	1.78	0.15	0.38	19.26
PCP-SAFT**	4.94245	3.74834	192.542	1	2.4549			3.24	1.48	0.13	0.42	19.39

[a] Critical temperature T_C, critical pressure p_C, acentric factor ω. Star denotes parameters developed by Aminian et al. [11].

[b] L, M and N parameters for the modified SRK and volume correction c.

[c] C_1, C_2, and C_3 parameters of the Mathias-Copeman α-function.

[d] Segment number m, segment diameter σ, energy parameter ε/k_b, number of dipoles n_μ, and dipole moment μ. Double star denotes parameters developed by Vinš et al. [8].

Table S10
Complete set of fitted parameters for various EOS and AARD for **liquid heat capacity optimization**. For EOS with subscript LCP (loose critical point), the critical properties can be parameters in the fitting procedure that lie outside the experimental uncertainties for the critical properties.

EOS	parameter of EOS							100 AARD				
[a]	T_C / K	p_C / MPa	ω / -					Over-all	ρ	p^{sat}	C_p	c
LKP	507.80	1.939	0.4450					9.95	11.36	2.57	2.55	11.56
LKP_{LCP}	504.56	2.282	0.4606					25.70	32.78	3.81	2.81	12.08
LKP-SJT1	505.54	1.795	0.5106					8.73	8.16	27.06	0.60	5.59
$LKP\text{-}SJT1_{LCP}$	500.08	1.740	0.5106					8.73	8.16	27.06	0.60	5.59
LKP-SJT2	506.65	1.811	0.5106					8.06	7.18	27.74	0.60	5.47
$LKP\text{-}SJT2_{LCP}$	519.68	1.261	0.5106					8.06	7.18	27.74	0.60	5.47
PR	508.80	1.897	0.6487					9.62	5.92	49.29	1.59	11.74
PR_{LCP}	539.24	1.428	0.6500					25.95	23.05	86.10	1.40	20.75
PR*	513.32	1.863	0.4351					4.79	2.05	14.46	5.74	15.28
SRK	508.80	1.958	0.5841					6.57	2.99	34.33	1.54	14.26
SRK_{LCP}	536.05	1.604	0.5838					24.93	22.99	77.75	1.37	17.82
[b]				L / -	M / -	N / -	c / cm^3 mol^{-1}					
PR-TWU-C	508.80	1.782	0.4284	2.09875	1.04282	0.36808	−24.0806	15.90	12.14	64.08	0.13	18.30
$PR\text{-}TWU\text{-}C_{LCP}$	521.63	1.280	0.5882	2.29403	1.19939	0.31169	−14.1673	28.63	33.52	18.11	0.10	25.78
[c]				C_1 / -	C_2 / -	C_3 / -						
SRK-MC	508.80	1.782	0.6138	1.52525	−0.81700	1.12866		13.77	11.18	49.90	0.33	15.34
$SRK\text{-}MC_{LCP}$	533.17	1.200	0.3972	1.49161	−0.68463	0.91733		40.08	41.63	84.07	0.20	28.80
[d]	m / -	σ / Å	ε/k_b / K	n_μ / -	μ / D							
PCP-SAFT	4.93938	4.32365	199.999	1	2.4949			29.23	31.87	61.60	0.17	10.62
PCP-SAFT**	4.94245	3.74834	192.542	1	2.4549			3.24	1.48	0.13	0.42	19.39

[a] Critical temperature T_C, critical pressure p_C, acentric factor ω. Star denotes parameters developed by Aminian et al. [11].

[b] L, M and N parameters for the modified SRK and volume correction c.

[c] C_1, C_2, and C_3 parameters of the Mathias-Copeman α-function.

[d] Segment number m, segment diameter σ, energy parameter ε/k_b, number of dipoles n_μ, and dipole moment μ. Double star denotes parameters developed by Vinš et al. [8].

Table S11
Complete set of fitted parameters for various EOS and AARD for **speed of sound optimization**. For EOS with subscript LCP (loose critical point), the critical properties can be parameters in the fitting procedure that lie outside the experimental uncertainties for the critical properties.

EOS	parameter of EOS							100 AARD				
[a]	T_C / K	p_C / MPa	ω / -					Over-all	ρ	p^{sat}	C_p	c
LKP	508.80	1.782	0.5229					11.52	8.72	52.40	5.87	4.90
LKP_{LCP}	509.45	1.463	0.5092					13.55	11.34	55.95	5.04	4.17
LKP-SJT1	506.02	1.908	0.5813					11.25	9.38	49.18	2.38	3.08
$LKP\text{-}SJT1_{LCP}$	502.38	1.500	0.5813					11.25	9.38	49.18	2.38	3.08
LKP-SJT2	506.71	1.856	0.5801					10.51	8.37	49.34	2.31	2.96
$LKP\text{-}SJT2_{LCP}$	534.95	1.549	0.5801					10.51	8.37	49.34	2.31	2.96
PR	508.80	1.970	0.6500					12.32	9.90	47.62	1.70	11.11
PR_{LCP}	540.00	2.600	0.5894					33.59	37.74	67.24	2.13	5.86
PR*	513.32	1.863	0.4351					4.79	2.05	14.46	5.74	15.28
SRK	508.80	1.970	0.6500					7.09	2.14	49.73	2.01	13.15
SRK_{LCP}	540.00	2.600	0.6389					23.69	23.22	75.38	1.67	6.40
[b]				L / -	M / -	N / -	c / cm^3 mol^{-1}					
PR-TWU-C	505.00	1.970	0.4284	1.00103	1.10445	2.39063	9.9932	21.84	18.71	73.79	19.10	6.81
$PR\text{-}TWU\text{-}C_{LCP}$	540.00	2.600	0.5359	1.18429	1.21648	1.52903	9.9548	44.29	49.04	80.12	19.55	3.13
[c]				C_1 / -	C_2 / -	C_3 / -						
SRK-MC	505.00	1.970	0.5028	2.00000	−1.17322	−1.99995		8.94	1.42	66.05	17.64	10.99
$SRK\text{-}MC_{LCP}$	528.06	2.600	0.6271	1.99951	−1.53831	−1.99365		26.76	26.06	69.92	19.70	5.65
[d]	m / -	σ / Å	ε/k_b / K	n_μ / -	μ / D							
PCP-SAFT	4.99999	4.31077	200.000	1	2.8000			29.67	32.02	65.95	0.90	9.95
PCP-SAFT**	4.94245	3.74834	192.542	1	2.4549			3.24	1.48	0.13	0.42	19.39

[a] Critical temperature T_C, critical pressure p_C, acentric factor ω. Star denotes parameters developed by Aminian et al. [11].

[b] L, M and N parameters for the modified SRK and volume correction c.

[c] C_1, C_2, and C_3 parameters of the Mathias-Copeman α-function.

[d] Segment number m, segment diameter σ, energy parameter ε/k_b, number of dipoles n_μ, and dipole moment μ. Double star denotes parameters developed by Vinš et al. [8].

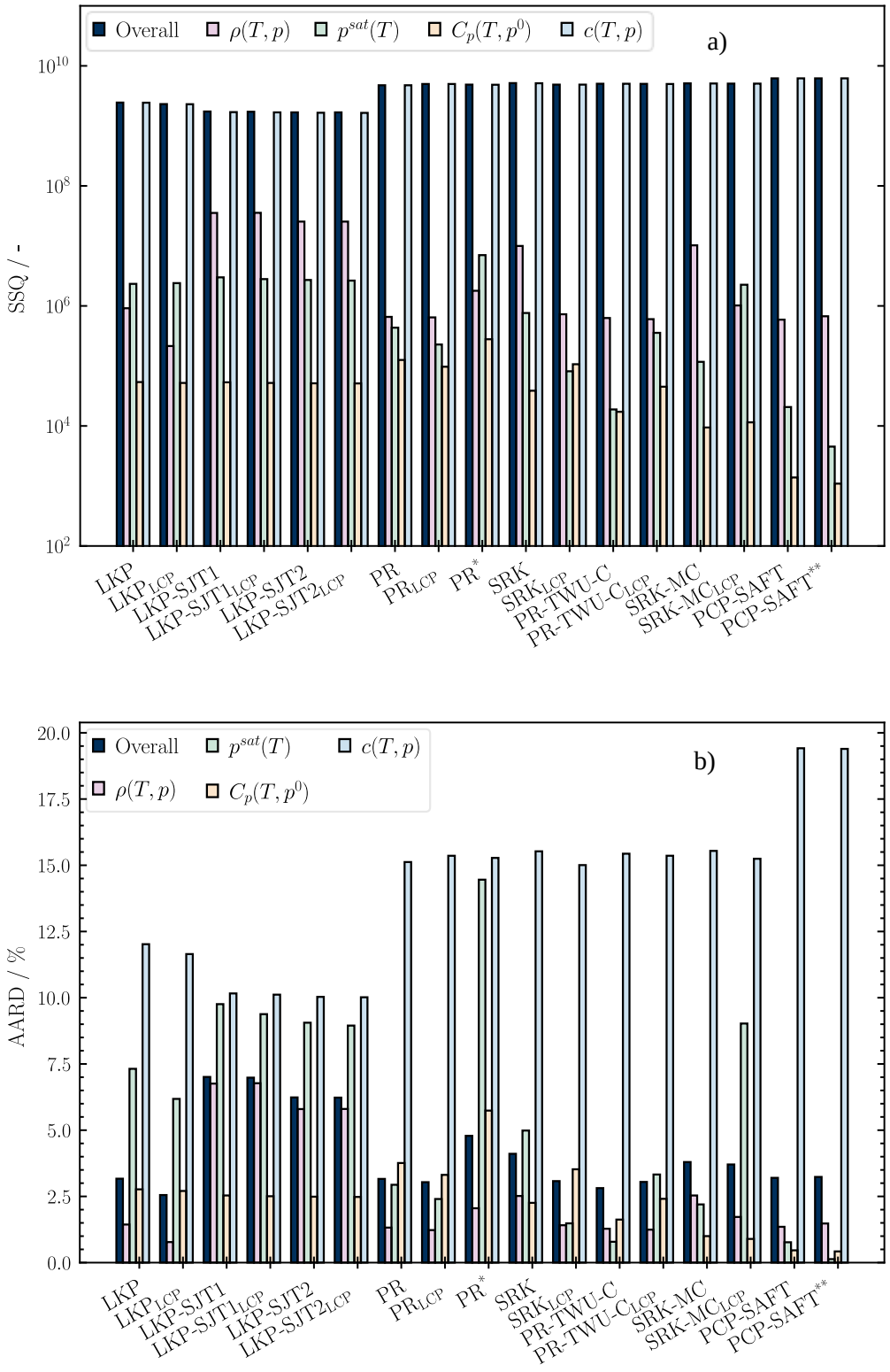

Figure S5. Full set of overall and individual-property SSQ (a) and AARD (b) values of HFE-7300 described with various EOS with parameters obtained through overall optimization. *Parameters developed by Aminian et al. [11] and **parameters developed by Vinš et al. [8].

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