

Modeling the thermal conductivity of hydrofluorocarbons, hydrofluoroolefins and their binary mixtures using residual entropy scaling and cubic-plus-association equation of state

Supplementary material

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S1. Dilute gas viscosity and thermal conductivity

The dilute gas viscosity is obtained from

$$\eta^{\circ} = \frac{5}{16} \left(\frac{mk_{\text{B}}T}{\pi} \right)^{\frac{1}{2}} \frac{1}{\sigma^2 \Omega^{(2,2)*}} \quad (\text{S1-1})$$

where m is the molecular mass, k_{B} is the Boltzmann constant, σ is one of the Lennard-Jones parameters, and $\Omega^{(2,2)*}$ is a collision integral.

For the binary mixture,

$$\eta_{\text{mix}}^{\circ} = \frac{1 + Z_{\eta}}{X_{\eta} + Y_{\eta}} \quad (\text{S1-2})$$

where the parameters X_{η} , Y_{η} , Z_{η} is given by

$$X_{\eta} = \frac{x_1^2}{\eta_1^{\circ}} + \frac{2x_1x_2}{\eta_{12}^{\circ}} + \frac{x_2^2}{\eta_2^{\circ}} \quad (\text{S1-3})$$

$$Y_{\eta} = \frac{3}{5} A^* \left\{ \frac{x_1^2}{\eta_1^{\circ}} \frac{m_1}{m_2} + \frac{2x_1x_2}{\eta_{12}^{\circ}} \frac{(m_1 + m_2)^2}{4m_1m_2} \frac{(\eta_{12}^{\circ})^2}{\eta_1^{\circ}\eta_2^{\circ}} + \frac{x_2^2}{\eta_2^{\circ}} \frac{m_2}{m_1} \right\} \quad (\text{S1-4})$$

$$Z_{\eta} = \frac{3}{5} A^* \left\{ x_1^2 \frac{m_1}{m_2} + 2x_1x_2 \left[\frac{(m_1 + m_2)^2}{4m_1m_2} \left(\frac{\eta_{12}^{\circ}}{\eta_1^{\circ}} + \frac{\eta_{12}^{\circ}}{\eta_2^{\circ}} \right) - 1 \right] + x_2^2 \frac{m_2}{m_1} \right\} \quad (\text{S1-5})$$

in which x_i denotes the molar fractions of components i , m_i denotes the molecular mass of component i , and η_i° denotes the dilute gas viscosity of components i . And the binary interaction dilute gas viscosity

$$\eta_{12}^{\circ} = \frac{5}{16} \left(\frac{2m_1m_2k_{\text{B}}T}{\pi(m_1 + m_2)} \right)^{\frac{1}{2}} \frac{1}{\sigma_{12}^2 \Omega^{(2,2)*}} \quad (\text{S1-6})$$

where the subscript '12' means the property of binary mixture of components 1 and 2.

The dilute gas thermal conductivity is represented by the sum of the translational and internal terms,

$$\lambda^{\circ} = \lambda^{\circ, \text{tr}} + \lambda^{\circ, \text{int}} \quad (\text{S1-7})$$

The translational term

$$\lambda^{\circ, \text{tr}} = \lambda^{\circ, \text{CE}} = \eta^{\circ} \cdot \frac{15R}{4M} = \frac{75}{64} \left(\frac{k_{\text{B}}^3 T}{\pi m} \right)^{\frac{1}{2}} \frac{1}{\sigma^2 \Omega^{(2,2)*}} \quad (\text{S1-8})$$

The internal term

$$\lambda^{\circ, \text{int}} = f^{\text{int}} \eta^{\circ} \cdot \frac{c_p^{\circ} - 2.5R}{M} \quad (\text{S1-9})$$

For the mixtures, the translational term

$$\lambda_{\text{mix}}^{\text{o, tr}} = 4 \cdot \frac{\begin{vmatrix} L_{11} & L_{12} & x_1 \\ L_{21} & L_{22} & x_2 \\ x_1 & x_2 & 0 \end{vmatrix}}{\begin{vmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{vmatrix}} \quad (\text{S1-10})$$

where the relevant determinant elements, L_{ij} is given by

$$L_{ii} = -\frac{4x_i^2}{\lambda_i^{\text{o, tr}}} - \sum_{\substack{k=1 \\ k \neq i}}^2 \frac{2x_i x_k \left[\frac{15}{2} m_i^2 + \frac{25}{4} m_k^2 - 3m_k^2 B^* + 4m_i m_k A^* \right]}{(m_i + m_k)^2 A^* \lambda_{ik}^{\text{o, tr}}} \quad (\text{S1-11})$$

$$L_{ij} = \frac{2x_i x_j m_i m_j}{(m_i + m_j)^2 A^* \lambda_{ij}^{\text{o, tr}}} \left(\frac{55}{4} - 3B^* - 4A^* \right) \quad (\text{S1-12})$$

in which $\lambda_i^{\text{o, tr}}$ is the thermal conductivity of components i , $\lambda_{ij}^{\text{o, tr}}$ is the binary interaction thermal conductivity. And the binary interaction thermal conductivity

$$\lambda_{ij}^{\text{o, tr}} = \frac{75}{64} \left(\frac{(m_i + m_j) k_B^3 T}{2\pi m_i m_j} \right)^{\frac{1}{2}} \frac{1}{\sigma_{ij}^2 \Omega^{(2,2)*}} \quad (\text{S1-13})$$

The internal term

$$\lambda_{\text{mix}}^{\text{o, int}} = \frac{x_1 \lambda_1^{\text{o, int}}}{x_1 + x_2 \cdot \frac{\lambda_1^{\text{o, tr}}}{\lambda_{12}^{\text{o, tr}}}} + \frac{x_2 \lambda_2^{\text{o, int}}}{x_1 \cdot \frac{\lambda_2^{\text{o, tr}}}{\lambda_{12}^{\text{o, tr}}} + x_2} \quad (\text{S1-14})$$

A^* and B^* in the formulations above are given by the recurrence relations among the reduced collision integrals,

$$A^* = \frac{\Omega^{(2,2)*}(T^*)}{\Omega^{(1,1)*}(T^*)} \quad (\text{S1-15})$$

$$B^* = \frac{5\Omega^{(1,2)*}(T^*) - 4\Omega^{(1,3)*}(T^*)}{\Omega^{(1,1)*}(T^*)} \quad (\text{S1-16})$$

And the collision integrals are calculated using the correlations proposed by Neufeld et al. [31]

$$\Omega^{(l,s)*} = A \cdot (T^*)^{-B} + C \cdot \exp(-DT^*) + E \cdot \exp(-FT^*) + G \cdot \exp(-HT^*) \quad (\text{S1-17})$$

where A to H are coefficients and given in Table S1, and T^* is the reduced temperature,

$$T^* = \frac{k_B T}{\varepsilon} \quad (\text{S1-18})$$

in which ε is a Lennard-Jones parameter. The values of Lennard-Jones parameters for each fluid are given in Table S2. The combination rules for Lennard-Jones parameters are applied for σ_{ij} and ε_{ij} :

$$\sigma_{ij} = (\sigma_i + \sigma_j) / 2 \quad (\text{S1-19})$$

$$\varepsilon_{ij} = (\varepsilon_i \varepsilon_j)^{1/2} \quad (\text{S1-20})$$

Table S1. Coefficients for Eq. (S1-17) [31]

(l, s)	A	B	C	D	E	F	G	H
(1, 1)	1.06036	0.15610	0.19300	0.47635	1.03587	1.52996	1.76474	3.89411
(1, 2)	1.00220	0.15530	0.16105	0.72751	0.86125	2.06848	1.95162	4.84492
(1, 3)	0.96573	0.15611	0.44067	1.52420	2.38981	5.08063	-	-
(2, 2)	1.16145	0.14874	0.52487	0.7732	2.16178	2.43787	-	-

Table S2. Lennard-Jones parameters

	ε / k (K)	σ (nm)
R23	243.91	0.4278
R32	289.65	0.4098
R125	237.077	0.5235
R134a	241.1846	0.522947
R143a	301.76	0.4827
R152a	354.84	0.46115
R161	320.39	0.4457
R227ea	289.34	0.5746
R236ea	318.33	0.5604
R236fa	307.24	0.5644
R245ca	355.41	0.5131
R245fa	258.15	0.588
R1234yf	275	0.531
R1234ze(E)	340	0.500
R1243zf	299.3171	0.497499

S2. Residual entropy derived from the CPA equation of state

The residual entropy is derived using the CPA equation of state

$$\begin{aligned}
 s^{\text{res}}(T, v) &= s^{\text{ig}}(T, v) - s(T, v) = \int_{\infty}^v \left[\frac{R}{v} - \left(\frac{\partial p}{\partial T} \right)_v \right] dv \\
 &= R \cdot \ln \frac{v}{v-b} + \frac{a_0}{b} \cdot \left(\frac{d\alpha}{dT} \right) \cdot \ln \frac{v}{v+b} \\
 &\quad + R \cdot \sum_i x_i \sum_{S_i} \left(\ln X_{S_i} + \frac{1-X_{S_i}}{2} \right) + RT \cdot \sum_i x_i \sum_{S_i} \left[\left(\frac{1}{X_{S_i}} - \frac{1}{2} \right) \left(\frac{\partial X_{S_i}}{\partial T} \right)_v \right]
 \end{aligned} \tag{S2-1}$$

where b is the co-volume parameter, a_0 is the energy parameter, α is a temperature-dependent parameter of which the expression is given by Yang et al. [30], and X_{S_i} is the association fraction defined as the molar fraction of molecules of component i that are not bonded at site S .

For the mixture, the parameters a and b are obtained using the van der Waals mixing rules:

$$a_0 = \sum_i \sum_j x_i x_j a_{ij}, \quad a_{ij} = \sqrt{a_i a_j} (1 - k_{ij}), \quad b = \sum_i x_i b_i \tag{S2-2}$$

where k_{ij} is the binary interaction parameter.

Elliot combining rule yields the association strength between sites on the molecules of components i and j

$$A_{ij} = \sqrt{A_i A_j} \tag{S2-3}$$

The values of parameters of the CPA equation of state are given by Refs. [7, 9] and listed in Tables S3 and S4 for the readers' convenience.

Table S3. Parameters of the CPA equation of state [7, 9]

Fluid	$10^5 b$ ($\text{m}^3 \cdot \text{mol}^{-1}$)	a_0 ($\text{Pa} \cdot \text{m}^6 \cdot \text{mol}^{-1}$)	m	ε ($\text{J} \cdot \text{mol}^{-1}$)	β ($\text{m}^3 \cdot \text{mol}^{-1}$)
R23	3.72752	0.310227	0.850471	6446.10	0.218766
R32	3.31389	0.298281	1.00235	7050.57	0.404758
R125	6.12710	0.602367	1.22687	3186.05	0.945557
R134a	5.73706	0.586692	1.28643	4571.58	0.802541
R143a	5.47754	0.499228	1.08849	5499.52	0.566483
R152a	5.02492	0.553875	0.759238	9304.95	0.150949
R161	4.58374	0.462490	1.07600	4598.28	0.862253
R227ea	8.33785	0.957174	0.806388	10206.9	0.063442
R236ea	7.87549	0.952849	1.18922	6607.66	0.321606
R236fa	8.06688	0.899544	1.42352	3556.38	1.20265
R245ca	7.50733	0.982583	1.29516	4525.52	0.793822
R245fa	7.58998	0.901422	1.53722	1636.58	4.02639
R1234yf	6.95371	0.712326	1.33291	1280.73	4.65539
R1234ze(E)	6.82823	0.752873	1.30929	2370.35	1.86251
R1243zf	6.66495	0.697543	1.25798	2415.93	2.21331

Table S4. Binary interaction parameter [7, 9]

Mixtures	k_{ij}	Mixtures	k_{ij}
R32 + R125	-6.25×10^{-5}	R125 + R1234yf	2.75×10^{-3}
R32 + R134a	0	R125 + R1234ze(E)	0
R32 + R1234yf	5.49×10^{-2}	R134a + R1234yf	2.46×10^{-2}
R32 + R1243zf	5.49×10^{-2}	R134a + R1234ze(E)	0
R125 + R134a	-1.94×10^{-3}	R143a + R1234yf	7.66×10^{-3}
R125 + R143a	-1.88×10^{-4}	R143a + R1234ze(E)	0
R125 + R152a	-3.88×10^{-2}	R1234yf + R1234ze(E)	0

S3. Ideal gas heat capacity

The ideal gas heat capacity is obtained by

$$\frac{c_p^0}{R} = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 \quad (\text{S3})$$

where the coefficients a_i are given in Table S5.

Table S5. Coefficients for Eq. (S3)

	a_0	$10^2 a_1$	$10^5 a_2$	$10^8 a_3$	$10^{11} a_4$
R23	3.690067	-0.13726	5.485254	-8.994197	4.578684
R32	4.721533	-1.19860	6.808847	-8.786923	3.805931
R125	3.207169	2.94935	0.235601	-3.920593	2.402037
R134a	1.765311	3.76180	-4.172453	4.136405	-1.773341
R143a	1.654150	3.11302	-1.650299	-0.414117	0.520793
R152a	3.354206	1.09966	2.497172	-2.779587	-0.004748
R161	4.954945	-1.10461	9.885696	-14.413032	6.990287
R227ea	3.680370	4.84744	-0.651654	-5.735809	3.975835
R236ea	7.968190	1.07927	9.429026	-18.405154	10.193112
R236fa	6.857480	2.27351	2.258328	-3.055435	1.843099
R245ca	3.371949	2.94506	6.738303	-17.519707	10.903392
R245fa	3.723243	3.75012	-0.947419	-0.911439	0.428942
R1234yf	2.323997	3.42897	1.799669	-9.366661	6.708448
R1234ze(E)	0.562885	6.94027	-16.585939	25.210613	-15.016428
R1243zf	-3.138878	7.06584	-9.631833	4.402524	2.753933

S4. Overview of the experimental data

Table S6

Overview of experimental thermal conductivity data for pure fluids

Source	T / K	p / MPa	Phase ^a	N^b		
				reported	selected	near-critical
R23	192 to 455	0.1 to 39.3	-	570	320	41
1975 Geller [33]	192 to 269	5 to 19.7	L	75	12	-
1976 Chaikovskiy [34]	283 to 375	0.1 to 4	G	28	18	2
1976 Chaikovskiy [34]	192 to 292	5 to 39.3	L	126	59	4
1976 Chaikovskiy [34]	313 to 434	5 to 39.3	SC	66	24	6
1976 Geller [35]	192 to 270	5 to 39.3	L	75	18	-
1977 Shestova [36]	309 to 453	0.2 to 4.4	G	45	45	4
1977 Shestova [36]	316 to 455	5.4	SC	8	8	2
1977 Zvetkob [37]	307 to 423	0.1	G	10	8	-
1981 Makita [38]	283 to 373	0.1 to 4.6	G	85	84	11
1981 Makita [38]	313 to 373	5 to 7	SC	30	22	12
1988 Potapov [39]	213 to 269	0.1 to 39.2	L	22	22	-
R32	223 to 466	0.1 to 50	-	1017	999	14
1993 Papadaki b [40]	229 to 303	0.1 to 1.9	Lsat	10	9	-
1994 Grebenkov [41]	275 to 351	1.7 to 10	L	72	68	10
1994 Grebenkov [41]	362 to 403	8.3 to 12.9	SC	24	24	2
1995 Assael [42]	253 to 313	0.6 to 17.6	L	27	27	-
1995 Ro [43]	223 to 323	2 to 25	L	24	24	-
1995 Tanaka [44]	283 to 333	0.1 to 3.9	G	53	53	-
1996 Gross [45]	265 to 345	0.1 to 4	G	43	43	-
1996 Gross [45]	233 to 334	0.2 to 6.2	L	37	37	2
1996 Yata [46]	253 to 324	1.9 to 30	L	27	27	-
1997 Ro [47]	233 to 323	2 to 20	L	48	48	-
1997 Sun [48]	287 to 313	0.8 to 1.9	G	20	7	-
2001 Le Neindre a [49]	299 to 466	0.1 to 5	G	109	109	-
2001 Le Neindre a [49]	299 to 338	3 to 50	L	206	206	-
2001 Le Neindre a [49]	353 to 465	6 to 50	SC	298	298	-
2001 Tomimura [50]	243 to 333	0.3 to 3.9	Lsat	19	19	-
R125	225 to 513	0.04 to 36	-	2041	1673	90
1990 Fellows [51]	307 to 332	1.7 to 3.0	L	6	6	2
1992 Asambaev [52]	250 to 290	1.2 to 5.1	L	12	5	-
1992 Wilson [53]	239 to 333	0.1	G	3	3	-
1992 Wilson [53]	298	1.4	Lsat	4	1	-
1993 Papadaki b [40]	225 to 306	0.1 to 1.7	Lsat	7	7	-
1994 Grebenkov [41]	295 to 336	1.7 to 11	L	40	40	4
1994 Grebenkov [41]	349 to 403	4.6 to 10	SC	34	34	4
1994 Tsvetkov [54]	226 to 290	0.1 to 1.1	Lsat	16	11	-

Source	T / K	p / MPa	Phase ^a	N^b		
				reported	selected	near-critical
1995 Assael [42]	253 to 313	1.2 to 16	L	20	20	-
1995 Tanaka [44]	283 to 333	0.1 to 2	G	51	51	-
1995 Tsvetkov [55]	237 to 349	0.1 to 0.5	G	19	13	-
1995 Tsvetkov [55]	228	4.1	L	11	1	-
1996 Gao [56]	233 to 334	2 to 30	L	32	24	1
1996 Yata [46]	257 to 305	1.1 to 30.9	L	24	24	-
1997 Assael [57]	273 to 313	0.2 to 1.1	G	17	17	-
1997 Ro [47]	231 to 324	2 to 20	L	48	48	2
1997 Sun [48]	256 to 330	0.2 to 2.5	G	17	15	1
1999 Jeong [58]	231 to 324	2 to 20	L	24	24	1
1999 Le Neindre a [59]	297 to 513	0.1 to 3	G	54	54	-
1999 Le Neindre a [59]	299 to 328	2.3 to 36	L	234	175	1
1999 Le Neindre a [59]	375 to 513	4 to 36	SC	352	263	-
2001 Tomimura [50]	243 to 333	0.2 to 3.1	Lsat	19	19	2
2006 Perkins [60]	232 to 392	0.04 to 3.5	G	519	498	16
2006 Perkins [60]	232 to 334	1.3 to 35	L	320	184	20
2006 Perkins [60]	352 to 392	3.6 to 31.9	SC	158	136	36
R134a	248 to 533	0 to 40	-	7529	6271	1096
1989 Richard [61]	303 to 343	0	G	5	5	-
1990 Fellows [39]	303 to 333	0.1	G	5	4	-
1990 Fellows [39]	312 to 342	1 to 2.1	L	8	8	-
1990 Gross [62]	274 to 354	0.3 to 2.7	Gsat	5	5	-
1990 Gross [62]	262 to 354	0.2 to 2.7	Lsat	13	13	-
1990 Ruvinskii [63]	253 to 400	0.1 to 3.1	G	17	13	1
1990 Ruvinskii [63]	253 to 362	0.7 to 8.9	L	27	25	3
1991 Tanaka [64]	293 to 353	0.1 to 2	G	33	31	-
1991 Ueno [65]	253 to 293	0.1	G	34	15	-
1992 Asambaev [52]	252 to 297	0.7 to 10.4	L	22	9	-
1992 Gross a [66]	274 to 354	0.1 to 1.8	G	40	29	-
1992 Gross a [66]	253 to 363	0.1 to 6.1	L	46	42	1
1992 Laesecke [67]	252 to 393	0.1 to 4	G	132	68	4
1992 Laesecke [67]	263 to 369	1.7 to 39.8	L	62	27	2
1992 Laesecke [67]	393	4.4 to 6	SC	21	10	10
1992 Lavrenchenko [68]	253 to 400	0.1 to 3.1	G	17	13	1
1992 Lavrenchenko [68]	253 to 362	0.7 to 8.9	L	27	24	3
1992 Perking [69]	263 to 303	0.7 to 5.2	L	76	52	-
1993 Papadaki a [70]	252 to 307	0.1 to 0.9	Lsat	9	7	-
1993 Yamamoto [71]	273 to 343	0.1 to 1.3	G	38	25	-
1994 Grebenkov [41]	293 to 363	1 to 19.6	L	48	48	-
1994 Grebenkov [41]	378 to 401	9.8 to 19.6	SC	17	16	-
1994 Gurova [72]	250 to 270	0.1	L	14	5	-

Source	T / K	p / MPa	Phase ^a	N^b		
				reported	selected	near-critical
1994 Kim [73]	248 to 323	2 to 20	L	25	20	-
1994 Tsvetkov [54]	248 to 290	0.1 to 0.5	Lsat	19	7	-
1995 Hammerschmidt [74]	303 to 463	0.1	G	5	5	-
1995 Liu [75]	248 to 298	0.1	G	26	11	-
1995 Ro [43]	248 to 323	2 to 20	L	24	19	-
1997 Assael [57]	273 to 333	0.1 to 1.3	G	19	19	-
1997 Gurova [76]	249 to 293	0.4 to 21.3	L	53	35	-
1999 Jeong [58]	248 to 323	2 to 20	L	25	20	-
1999 Le Neindre b [77]	454 to 533	0.1 to 4	G	52	20	-
1999 Le Neindre b [77]	299 to 355	2 to 40	L	208	184	-
1999 Le Neindre b [77]	374 to 533	5 to 40	SC	283	279	-
2000 Perkins [78]	250 to 450	0.02 to 4	G	2568	2373	95
2000 Perkins [78]	250 to 370	0.6 to 39.8	L	1601	1127	177
2000 Perkins [78]	390 to 450	4.2 to 39	SC	1153	999	208
2001 Tomimura [50]	248 to 333	0.1 to 1.7	Lsat	19	18	-
2009 Le Neindre [79]	299 to 516	0.1 to 4.1	G	118	113	63
2009 Le Neindre [79]	374 to 376	4 to 4.1	L	8	8	8
2009 Le Neindre [79]	374 to 405	4.1 to 6	SC	607	520	520
R143a	233 to 499	0.1 to 37.1	-	690	539	10
1996 Yata [46]	268 to 298	2.4 to 31.1	L	24	16	-
2001 Le Neindre b [80]	299 to 499	0.1 to 3.5	G	126	88	2
2001 Le Neindre b [80]	305 to 337	2.5 to 37	L	142	108	4
2001 Le Neindre b [80]	348 to 499	4 to 37.1	SC	375	308	4
2001 Lee [81]	233 to 299	2 to 20	L	23	19	-
R152a	250 to 510	0.03 to 45	-	2554	1734	239
1976 Slusarev [82]	253 to 373	4 to 40	L	36	21	1
1976 Slusarev [82]	393	20 to 40	SC	3	2	-
1977 Zvetkob [37]	264 to 418	0.1	G	11	10	-
1979 Slusarev [83]	254 to 377	10 to 40	L	43	24	-
1979 Slusarev [83]	254 to 356	0.1 to 2.5	Lsat	17	12	-
1979 Slusarev [83]	403 to 431	5 to 40	SC	23	9	2
1980 Afshar [84]	280 to 510	0.1	G	13	13	-
1982 Geller [85]	306 to 382	1.1 to 5.9	L	107	98	39
1988 Potapov [39]	313 to 344	0.1	L	6	6	-
1992 Gross a [66]	254 to 354	0.1 to 2.3	G	40	40	-
1992 Gross a [66]	253 to 363	0.2 to 6.2	L	44	37	-
1992 Gross b [86]	253 to 313	0.1 to 6.2	L	24	24	-
1992 Yata [87]	266 to 343	1.4 to 30.6	L	20	20	-
1992 Yin [88]	279 to 349	0.1	G	14	14	-
1993 Kim [89]	273 to 323	2.1 to 20.1	L	25	15	-

Source	T / K	p / MPa	Phase ^a	N^b		
				reported	selected	near-critical
1994 Grebenkov [41]	294 to 381	0.8 to 20	L	72	53	6
1994 Grebenkov [41]	398	15 to 20	SC	6	4	-
1994 Haynes [90]	251 to 414	0.03 to 4.3	G	758	600	40
1994 Haynes [90]	266 to 372	2.6 to 41.3	L	405	186	8
1994 Haynes [90]	411 to 412	4.6 to 6.5	SC	425	137	137
1995 Hammerschmidt [74]	303 to 463	0.1	G	5	5	-
1996 Tsvetkov [91]	253 to 300	7.9 to 8.1	L	11	5	-
1999 Gurova [92]	250 to 294	0.8 to 18	L	38	23	-
2002 Le Neindre [93]	305 to 456	0.1 to 4.5	G	48	46	-
2002 Le Neindre [93]	307 to 378	1 to 45	L	252	222	5
2002 Le Neindre [93]	391 to 455	5 to 41	SC	108	108	1
R161	236 to 381	0.1 to 5.2	-	370	361	29
2014 Yao [94]	236 to 377	0.1 to 4.5	G	199	199	7
2014 Yao [94]	244 to 375	0.1 to 4.9	Lsat	167	158	18
2014 Yao [94]	377 to 381	5.2	SC	4	4	4
R227ea	282 to 344	0.04 to 2.9	-	491	291	-
2001 Perkins [95]	282 to 334	0.04 to 0.4	G	439	239	-
2003 Baginskii [96]	294 to 344	1 to 2.9	L	52	52	-
R236ea	281 to 334	0.05 to 0.5	-	202	202	-
2001 Perkins [95]	281 to 334	0.05 to 0.5	G	202	202	-
R236fa	273 to 375	0.03 to 30	-	271	256	-
2001 Perkins [95]	281 to 343	0.03 to 0.5	G	169	169	-
2011 Pan [97]	273 to 375	1 to 30	L	102	87	-
R245ca	298 to 393	0.03 to 0.3	-	164	131	-
1999 Dohrn [98]	303 to 393	0.1	G	4	3	-
2001 Perkins [95]	298 to 335	0.03 to 0.3	G	160	128	-
R245fa	290 to 416	0.1 to 35.5	-	1530	555	3
1999 Dohrn [98]	333 to 382	0.1	G	4	4	-
1999 Geller [99]	290 to 376	0.1 to 1	G	26	9	-
1999 Geller [99]	309 to 390	0.2 to 1.8	Lsat	14	8	-
2000 Yata [100]	296 to 315	1.3 to 14.7	L	16	8	-
2004 Grebenkov [101]	300 to 316	0.1	G	69	10	-
2004 Grebenkov [101]	300 to 393	0.4 to 10	L	115	103	-
2006 Wang [102]	296 to 416	0.1 to 2.5	G	90	90	-
2006 Wang [102]	294 to 416	0.1 to 2.9	Lsat	58	43	3
2016 Perkins [103]	295 to 340	0.2 to 35.5	L	1138	280	-

Source	T / K	p / MPa	Phase ^a	N ^b		
				reported	selected	near-critical
R1234yf	244 to 344	0.1 to 21.7	-	801	744	-
2011 Perkins [104]	244 to 344	0.1 to 1.9	G	479	461	-
2011 Perkins [104]	244 to 344	0.8 to 21.7	L	311	273	-
2011 Perkins [104]	253 to 343	0.2 to 2	Lsat	11	10	-
R1234ze(E)	255 to 402	0.05 to 23.3	-	1301	1102	2
2009 Grebenkov [105]	255 to 402	0.05 to 3.6	G	84	83	2
2011 Perkins [104]	261 to 343	0.1 to 1.4	G	750	709	-
2011 Perkins [104]	261 to 343	0.4 to 23.3	L	452	301	-
2011 Perkins [104]	263 to 343	0.1 to 1.6	Lsat	15	9	-
R1243zf	314 to 406	0.9 to 6.1	-	35	35	-
2020 Kim b [106]	356 to 406	0.9 to 3.3	G	10	10	-
2020 Kim b [106]	314 to 375	2 to 6.1	L	25	25	-
Overall	192 to 533	0 to 50	-	19566	15213	1524

^a G: gas; Gsat: saturated gas; L: liquid; Lsat: saturated liquid; SC: supercritical.

^b Number of data which are (reported by the literature / selected in this work / distributed in the near-critical region).

Table S7

Overview of experimental thermal conductivity data for binary mixtures

Source	x_1	T / K	p / MPa	Phase ^a	N^b		
					reported	selected	near-critical
R32 + R125	0.19 to 0.88	233 to 428	0.1 to 30	-	466	453	22
1995 Tanaka [44]	0.19 to 0.82	283 to 298	0.1 to 1.2	G	69	69	-
1997 Ro [47]	0.44 to 0.88	233 to 324	2 to 20	L	120	119	4
1999 Gao [111]	0.43 to 0.87	233 to 293	2 to 30	L	60	48	-
2001 Geller [112]	0.7	255 to 410	0.1 to 3.7	G	50	50	6
2001 Tomimura [50]	0.55 to 0.83	243 to 333	0.3 to 3.9	Lsat	57	57	9
2017 Verba [113]	0.7	315 to 428	0.1 to 2	G	98	98	-
2020 Kim a [114]	0.5	304 to 366	1 to 3	G	6	6	2
2020 Kim a [114]	0.5	254 to 323	1.5 to 5.1	L	6	6	1
R32 + R134a	0.3 to 0.85	248 to 385	0.1 to 30	-	1476	1425	68
1995 Ro [43]	0.46 to 0.85	248 to 323	2 to 20	L	72	57	-
1999 Gao [111]	0.39 to 0.85	253 to 316	2 to 30	L	84	48	-
1999 Perkins [115]	0.3 to 0.7	256 to 347	0.1 to 0.6	G	999	999	-
1999 Perkins [115]	0.3 to 0.7	253 to 359	0.3 to 11.7	L	309	309	66
2020 Kim a [114]	0.5	325 to 385	1 to 3.1	G	6	6	2
2020 Kim a [114]	0.5	254 to 334	1.5 to 5	L	6	6	-
R32 + R1234yf	0.25 to 0.75	264 to 395	0.9 to 4	-	36	36	-
2020 Kim b [106]	0.25 to 0.75	315 to 395	0.9 to 2.8	G	16	16	-
2020 Kim b [106]	0.25 to 0.75	264 to 324	1.5 to 4	L	20	20	-
R32 + R1243zf	0.25 to 0.75	264 to 395	1 to 4	-	37	37	1
2020 Kim b [106]	0.25 to 0.75	325 to 395	1 to 4	G	17	17	-
2020 Kim b [106]	0.25 to 0.75	264 to 334	1.4 to 4	L	20	20	1
R125 + R134a	0.19 to 0.79	248 to 387	0.1 to 20	-	1201	1160	24
1999 Jeong [58]	0.19 to 0.79	248 to 324	2 to 20	L	96	76	4
1999 Perkins [115]	0.3 to 0.7	257 to 343	0.1 to 0.6	G	815	815	-
1999 Perkins [115]	0.3 to 0.7	252 to 345	0.5 to 9.9	L	278	257	17
2020 Kim a [114]	0.5	325 to 387	1 to 3.7	G	6	6	2
2020 Kim a [114]	0.5	255 to 323	1 to 3	L	6	6	1
R125 + R143a	0.41	255 to 372	0.1 to 3.8	-	162	162	25
2001 Geller [112]	0.41	255 to 372	0.1 to 2.6	G	34	34	2
2008 Baginsky [116]	0.41	298 to 333	1.5 to 3.8	L	128	128	23
R125 + R152a	0.5	274 to 394	1 to 3.1	-	12	11	1
2019 Mylona [117]	0.5	336 to 394	1.1 to 3.1	G	6	6	-
2019 Mylona [117]	0.5	274 to 314	1 to 3.1	L	6	5	1

Source	x_1	T / K	p / MPa	Phase ^a	N^b		
					reported	selected	near-critical
R125 + R1234yf	0.5	260 to 394	1.1 to 3.1	-	12	12	3
2019 Mylona [117]	0.5	335 to 394	1.3 to 3.1	G	6	6	2
2019 Mylona [117]	0.5	260 to 325	1.1 to 3	L	6	6	1
R125 + R1234ze(E)	0.5	263 to 395	1 to 3.1	-	12	12	3
2019 Mylona [117]	0.5	334 to 395	1.1 to 3	G	6	6	2
2019 Mylona [117]	0.5	263 to 324	1 to 3.1	L	6	6	1
R134a + R1234yf	0.5	255 to 385	1 to 3	-	12	12	2
2020 Kim a [114]	0.5	335 to 385	1 to 3	G	6	6	2
2020 Kim a [114]	0.5	255 to 324	1 to 3	L	6	6	-
R134a + R1234ze(E)	0.5	275 to 404	0.9 to 3.1	-	12	12	2
2019 Mylona [117]	0.5	344 to 404	0.9 to 3	G	6	6	2
2019 Mylona [117]	0.5	275 to 326	1 to 3.1	L	6	6	-
R143a + R1234yf	0.5	265 to 394	1.1 to 3.1	-	12	12	2
2019 Mylona [117]	0.5	334 to 394	1.1 to 3.1	G	6	6	2
2019 Mylona [117]	0.5	265 to 324	1.1 to 3.1	L	6	6	-
R143a + R1234ze(E)	0.5	265 to 404	0.9 to 3	-	12	12	1
2019 Mylona [117]	0.5	345 to 404	1 to 3	G	6	6	1
2019 Mylona [117]	0.5	265 to 324	0.9 to 3	L	6	6	-
R1234yf + R1234ze(E)	0.5	275 to 414	0.9 to 3	-	12	12	2
2019 Mylona [117]	0.5	355 to 414	0.9 to 2.9	G	6	6	2
2019 Mylona [117]	0.5	275 to 325	1.1 to 3	L	6	6	-
Overall	-	233 to 428	0.1 to 30	-	3474	3368	156

^a G: gas; Gsat: saturated gas; L: liquid; Lsat: saturated liquid; SC: supercritical.

^b Number of data which are (reported by the literature / selected in this work / distributed in the near-critical region).