



The International Association for the Properties of Water and Steam

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Release on the IAPWS Formulation 2021 for the Thermal Conductivity of Heavy Water

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This release replaces the thermal conductivity portion of the revised release of 2007 (IAPWS R4-84(2007)), and contains 11 pages, including this cover page.

This Revised Release has been authorized by the International Association for the Properties of Water and Steam (IAPWS) at its virtual meeting on 14-17 September, 2021. The members of IAPWS are: Australia, Britain and Ireland, Canada, the Czech Republic, Germany, Japan, New Zealand, Russia, Scandinavia (Denmark, Finland, Norway, Sweden), and the United States, and associate members Argentina and Brazil, China, Egypt, France, Greece, Israel, Italy, and Switzerland. The President at the time of adoption of this document was Prof. Masaru Nakahara of Japan.

Summary

The formulation provided in this Release is recommended for calculating the thermal conductivity of heavy water, which IAPWS defines as water whose hydrogen atoms are entirely the deuterium isotope (^2H or D) and whose oxygen isotopes have the same abundance as in ordinary water [1]. Further details about the formulation can be found in the article “New International Formulation for the Thermal Conductivity of Heavy Water” by M.L. Huber *et al.* [2]. This formulation provides the most accurate representation available at the time this Release was prepared for the thermal conductivity of the fluid phases of heavy water over a wide range of conditions.

Further information about this Release and other documents issued by IAPWS can be obtained from the Executive Secretary of IAPWS (Dr. R.B. Dooley, bdooley@iapws.org) or from <http://www.iapws.org>.

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1. Introductory Remarks

This release provides a correlating equation for the thermal conductivity of pure heavy water, D₂O, over an extended range of fluid states. A discussion of the background, development, and validation of this formulation is presented in Ref. [2].

Section 2 of this release contains the correlating equation, necessary constants, range of validity of the correlation, and estimates of the uncertainty of the correlation. Section 3 deals with the industrial application of the thermal-conductivity equation.

2. Recommended Correlating Equation

2.1. Nomenclature

T denotes absolute temperature on the International Temperature Scale of 1990

ρ denotes density

p denotes pressure

λ denotes thermal conductivity

μ denotes viscosity

c_p denotes isobaric specific heat capacity

c_v denotes isochoric specific heat capacity

2.2. Reference constants

The reference constants used in this formulation for temperature and density agree with the presently accepted values of the critical temperature, pressure, and density of heavy water recommended by IAPWS [3], while the reference constants for thermal conductivity and viscosity have no physical significance.

$$\text{reference temperature:} \quad T^* = 643.847 \text{ K} \quad (1)$$

$$\text{reference pressure:} \quad p^* = 21.6618 \text{ MPa} \quad (2)$$

$$\text{reference density:} \quad \rho^* = 356.0 \text{ kg m}^{-3} \quad (3)$$

$$\text{reference thermal conductivity:} \quad \lambda^* = 1 \times 10^{-3} \text{ W m}^{-1} \text{ K}^{-1} \quad (4)$$

$$\text{reference viscosity:} \quad \mu^* = 1 \times 10^{-6} \text{ Pa s} \quad (5)$$

$$\text{specific gas constant:} \quad R = 0.415 \ 151 \ 99 \text{ kJ kg}^{-1} \text{ K}^{-1} \quad (6)$$

2.3. Dimensionless variables

$$\text{temperature:} \quad \bar{T} = T / T^* \quad (7)$$

$$\text{pressure:} \quad \bar{p} = p / p^* \quad (8)$$

$$\text{density:} \quad \bar{\rho} = \rho / \rho^* \quad (9)$$

$$\text{thermal conductivity:} \quad \bar{\lambda} = \lambda / \lambda^* \quad (10)$$

$$\text{viscosity:} \quad \bar{\mu} = \mu / \mu^* \quad (11)$$

$$\text{isobaric heat capacity:} \quad \bar{c}_p = c_p / R \quad (12)$$

$$\text{heat-capacity ratio:} \quad \kappa = c_p / c_v \quad (13)$$

2.4. Range of validity

Equation (15) below is recommended for computation of the thermal conductivity for all thermodynamically stable fluid states in the following ranges of pressure p and temperature T :

$$\begin{aligned} 0 < p \leq p_t & \quad \text{and} \quad T_t \leq T \leq 825 \text{ K} \\ p_t \leq p \leq 250 \text{ MPa} & \quad \text{and} \quad T_m(p) \leq T \leq 825 \text{ K}. \end{aligned} \quad (14)$$

In the inequalities above, $T_m(p)$ is the pressure-dependent melting temperature, p_t is the triple-point pressure, and $T_t = 276.969 \text{ K}$ is the triple-point temperature as given in Ref. [4]. The density from the equation of state in Ref. [4] should be used to determine the densities used as input to Eq. (15) when the state point under consideration is defined by pressure and temperature or by other thermodynamic variables instead of density and temperature.

In addition, IAPWS makes the following statements about the extrapolation of Eq. (15) outside the range of validity given above:

- For vapor states at temperatures below the triple-point temperature [4] of 276.969 K and pressures less than or equal to the sublimation pressure, the thermal conductivity calculation is dominated by the dilute-gas term, and this behaves in a physically reasonable manner at least as low in temperature as 250 K.

- For stable fluid states outside the range of validity of Eq. (15) but within the range of validity of the Revised Release on the IAPWS Formulation 2017 for the Thermodynamic Properties of Heavy Water [3], the extrapolation behavior of Eq. (15) is physically reasonable.
- At high temperatures, the extrapolation of the dilute-gas portion of Eq. (15) is physically reasonable up to at least 2500 K.

2.5. Estimated uncertainty

The uncertainties in this formulation are summarized in Figure 1; they should be considered as estimates of an expanded uncertainty with a coverage factor of two. Since the thermal conductivity diverges at the critical point, the uncertainty may become larger near the critical point.

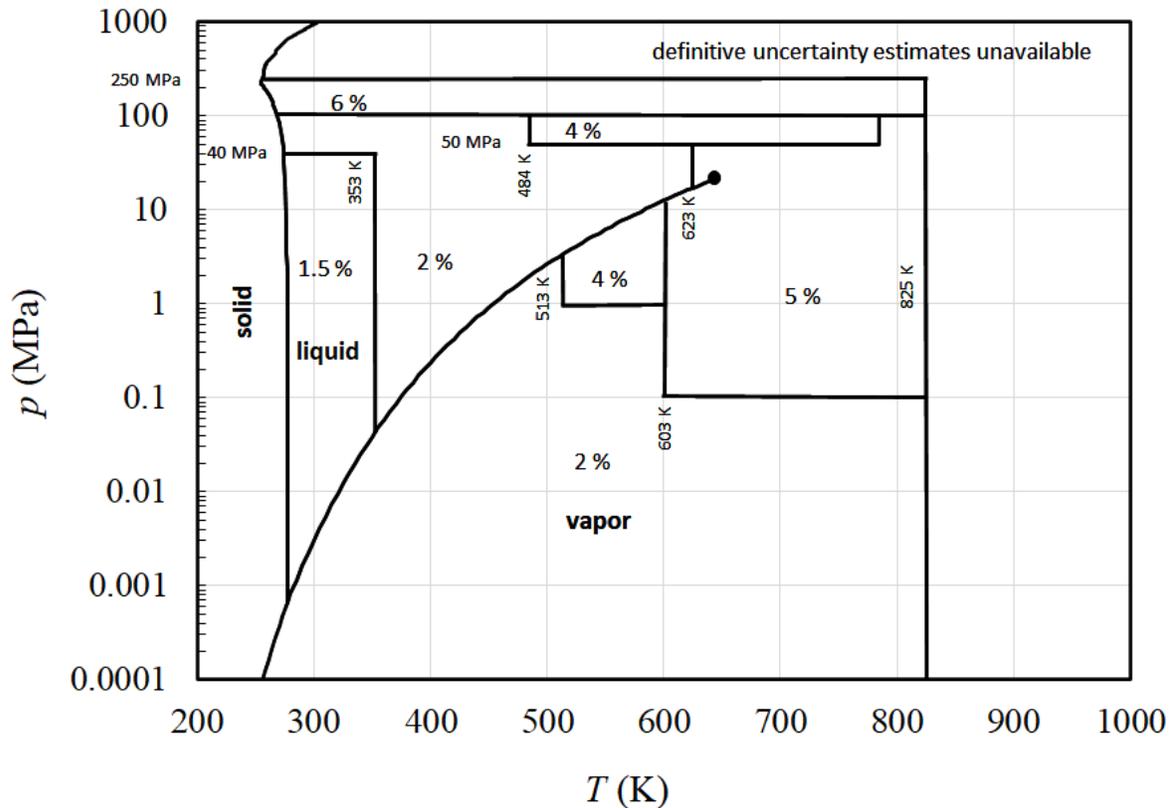


Figure 1. Estimated expanded uncertainty ($k=2$) of the correlating equation.

2.6. Correlating equation

The thermal conductivity is represented by the equation

$$\bar{\lambda} = \bar{\lambda}_0(\bar{T}) \times \bar{\lambda}_1(\bar{T}, \bar{\rho}) + \bar{\lambda}_2(\bar{T}, \bar{\rho}). \quad (15)$$

The first factor $\bar{\lambda}_0$ of the product in Eq. (15) represents the thermal conductivity in the dilute-gas limit and is given by

$$\bar{\lambda}_0(\bar{T}) = \sqrt{\bar{T}} \frac{1 + 3.3620798 \bar{T} - 1.0191198 \bar{T}^2 + 2.8518117 \bar{T}^3}{0.10779213 - 0.034637234 \bar{T} + 0.036603464 \bar{T}^2 + 0.0091018912 \bar{T}^3}. \quad (16)$$

The second factor $\bar{\lambda}_1$ of the product in Eq. (15) represents the contribution to thermal conductivity due to finite density:

$$\bar{\lambda}_1(\bar{T}, \bar{\rho}) = \exp \left[\bar{\rho} \sum_{i=0}^4 \left(\frac{1}{\bar{T}} - 1 \right)^i \sum_{j=0}^5 L_{ij} (\bar{\rho} - 1)^j \right], \quad (17)$$

with coefficients L_{ij} given in Table 1.

Table 1. Coefficients L_{ij} in Eq. (17) for $\bar{\lambda}_1(\bar{T}, \bar{\rho})$.

j i	0	1	2	3	4	5
0	1.509 335 76	-0.658 310 78	0.111 174 263	0.140 185 152	-0.065 622 772 2	0.007 851 552 13
1	2.841 471 5	-2.982 657 7	1.343 579 32	-0.599 233 641	0.281 163 37	-0.053 329 283 3
2	4.860 957 23	-6.197 844 68	2.209 418 67	0.224 691 518	-0.322 191 265	0.059 620 465 4
3	2.061 560 07	-3.486 124 56	1.479 623 09	0.625 101 458	-0.561 232 25	0.097 444 613 9
4	-2.061 056 87	0.416 240 028	2.925 245 13	-2.817 035 83	1.005 514 76	-0.127 884 416

2.7. Critical enhancement

The additive contribution $\bar{\lambda}_2$ in Eq. (15) represents the critical enhancement of the thermal conductivity. This additive contribution is defined over the entire range of states by

$$\bar{\lambda}_2(\bar{T}, \bar{\rho}) = \Lambda \frac{\bar{\rho} c_p \bar{T}}{\bar{\mu}} Z(y), \quad (18)$$

where Λ is a numerical constant. The function $Z(y)$ is defined by

$$Z(y) = \frac{2}{\pi y} \left\{ (1 - \kappa^{-1}) \arctan(y) + \kappa^{-1} y - \left[1 - \exp\left(\frac{-1}{y^{-1} + y^2 / 3\bar{\rho}^2}\right) \right] \right\}, \quad (19)$$

where $\kappa = c_p / c_v$ and

$$y = q_D \xi(\bar{T}, \bar{\rho}). \quad (20)$$

In Eq. (20), q_D is a reference wave number and ξ a correlation length, so that y is a dimensionless variable. To avoid numerical truncation issues in Eq. (19) for small values of y , the function $Z(y)$ is subject to the condition

$$Z(y) = 0 \text{ for } y < 1.2 \times 10^{-7}. \quad (21)$$

The correlation length ξ in Eq. (20) is to be calculated by the same procedure as that defined in the IAPWS Formulation 2020 for the Viscosity of Heavy Water [5,6]. Specifically,

$$\xi = \xi_0 \left(\frac{\Delta \bar{\chi}}{\Gamma_0} \right)^{\nu/\gamma} \quad (22)$$

in terms of $\Delta \bar{\chi}$ (≥ 0) defined by

$$\Delta \bar{\chi}(\bar{T}, \bar{\rho}) = \bar{\rho} \left[\zeta(\bar{T}, \bar{\rho}) - \zeta(\bar{T}_R, \bar{\rho}) \frac{\bar{T}_R}{\bar{T}} \right] \quad (23)$$

with

$$\zeta = \left(\frac{\partial \bar{\rho}}{\partial \bar{p}} \right)_{\bar{T}}, \quad (24)$$

where ξ_0, Γ_0, ν , and γ are constants.

When $\Delta \bar{\chi}$ calculated from Eq. (23) is less than zero, it must be set to zero for calculations to proceed.¹ The constants needed to compute the critical enhancement, $\bar{\lambda}_2$, are provided in Table 2.

Table 2. Critical-region constants.

Constant	Value
Λ	175.9870
q_D^{-1}	0.36 nm
ν	0.630
γ	1.239
ξ_0	0.13 nm
Γ_0	0.06
\bar{T}_R	1.5

¹ Due to the numerical implementation of the equation of state, the calculated singularity in the first derivative in Eq. (23) may not occur exactly at $T_c = T^*$ and $\rho_c = \rho^*$ as it should. Therefore, calculated values of $\bar{\lambda}_2$ may behave unphysically at points extremely close to the critical point (approximately within 0.01 kg m^{-3} of ρ_c on the critical isotherm). The formulation should be used with caution in this very small region.

For general and scientific use, the dimensionless isobaric heat capacity, \bar{c}_p , in Eq. (18), the heat-capacity ratio, κ , in Eq. (19), and the dimensionless isothermal compressibility, ζ , in Eq. (23) are to be calculated from the IAPWS Formulation 2017 for the Thermodynamic Properties of Heavy Water [3], while the dimensionless viscosity, $\bar{\mu}$, in Eq. (18) is to be calculated from Eq. (10) in the IAPWS Formulation 2020 for the Viscosity of Heavy Water [5].

Figure 2 shows the significance of the critical-enhancement contribution to the thermal conductivity at various temperatures and densities.

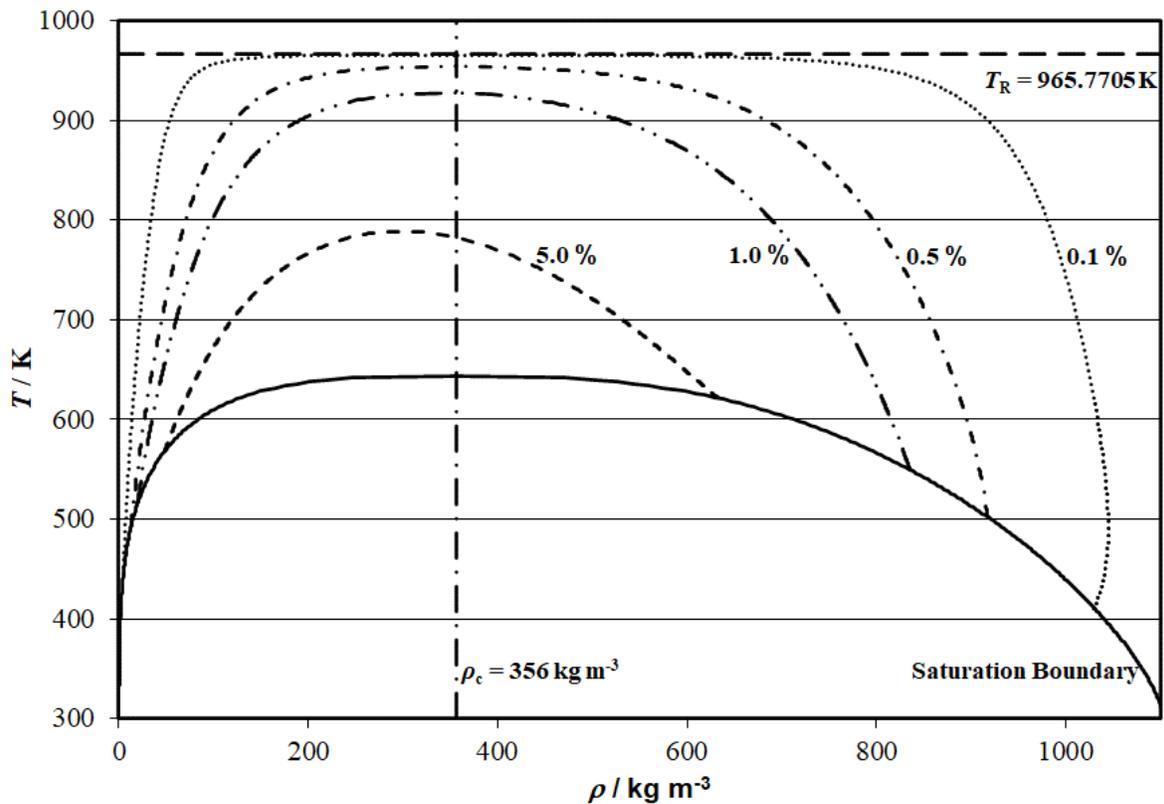


Figure 2. Contours in the temperature-density plane where the contribution from the critical enhancement $\bar{\lambda}_2$ to the total thermal conductivity $\bar{\lambda}$ equals 5%, 1%, 0.5%, and 0.1%.

2.8. Computer-program verification of the correlating equation

The following tables are provided to assist the user in computer-program verification. The thermal-conductivity values are calculated as a function of the tabulated temperatures and densities.

Table 3. Sample points for computer-program verification of the correlating equation, Eq. (15). At these points, $\bar{\lambda}_2 = 0$.

T (K)	ρ (kg m ⁻³)	λ (mW m ⁻¹ K ⁻¹)
298.15	0	17.7498
298.15	1104.5	599.557
298.15	1200	690.421
825.00	0	76.4492

Table 4. Sample points for computer-program verification of the correlating equation, Eq. (15), including the critical-enhancement contribution $\bar{\lambda}_2$. For all points, $\bar{\lambda}_0$ (644.10 K) = 52.149 66 and $T = 644.10$ K.

ρ (kg m ⁻³)	$\bar{\lambda}_1$	$\bar{\lambda}_2$	λ (mW m ⁻¹ K ⁻¹)
1	1.005 807 6	0.000 133 2	52.4527
106	1.791 564 9	9.912 756 7	103.342
256	3.390 704 3	217.787 846	394.612
306	3.963 958 7	594.662 792	801.382
356	4.518 682 1	1042.775 41	1278.423
406	5.041 459 0	407.922 272	670.833
456	5.529 512 3	135.240 705	423.603
750	8.598 246 1	6.450 078 1	454.846

3. Recommendations for Industrial Use

3.1. Industrial application of correlating equation

For industrial applications where greater computing speed is needed, the recommended formulation for calculating the thermal conductivity for industrial applications $\bar{\lambda}_1$ has a form similar to Eq. (15):

$$\bar{\lambda}_1 = \bar{\lambda}_0(\bar{T}) \times \bar{\lambda}_1(\bar{T}, \bar{\rho}) + \bar{\lambda}_{21}(\bar{T}, \bar{\rho}), \quad (25)$$

where the functions $\bar{\lambda}_0(\bar{T})$ and $\bar{\lambda}_1(\bar{T}, \bar{\rho})$ are identical to those specified in Eqs. (16) and (17), but where for industrial application we use

$$\bar{\lambda}_{21}(\bar{T}, \bar{\rho}) = \Lambda \frac{\bar{\rho} \bar{c}_p \bar{T}}{\bar{\mu}_0 \bar{\mu}_1} Z(q_D \xi_1). \quad (26)$$

The dimensionless background viscosity, $\bar{\mu}_0\bar{\mu}_1$, in Eq. (26) should be calculated from the recommended viscosity correlation for industrial application as described in the IAPWS Formulation 2020 for the Viscosity of Heavy Water [5], which does not include the critical enhancement of viscosity. In Eq. (26), the dimensionless isobaric heat capacity, \bar{c}_p , as well as the density derivative in Eq. (24) and the heat-capacity ratio, κ , in Eq. (19), are to be calculated with the Revised Release on the IAPWS Formulation 2017 for the Thermodynamic Properties of Heavy Water [3]. The function $\zeta(\bar{T}_R, \bar{\rho})$ in Eq. (23) is calculated from

$$\zeta(\bar{T}_R, \bar{\rho}) = \frac{1}{\sum_{i=0}^{10} A_i \bar{\rho}^i} \quad (27)$$

with coefficients A_i given in Table 5.

Table 5. Coefficients A_i in Eq. (27) for $\zeta(\bar{T}_R, \bar{\rho})$.

i	A_i
0	6.584 360
1	-5.362 300
2	-0.611 633
3	21.445 300
4	-45.055 900
5	54.050 400
6	-39.433 200
7	17.948 500
8	-4.916 820
9	0.739 039
10	-0.046 751

3.2. Estimated uncertainty of industrial equation

The uncertainty of the industrial equation results from three contributions: (1) the uncertainty of the recommended correlating equation for general and scientific use, illustrated in Figure 1, (2) the deviation caused by using the industrial equation for the viscosity, and (3) the approximation for the compressibility at the reference temperature T_R . Since the latter two contributions are much smaller than the first, the uncertainties shown in Figure 1 are applicable to the industrial equation except for a small region near the critical point, where deviations of the industrial equation become larger. This is illustrated in Figure 3 and exceeds 1.5% only for $T - T_c < 5$ K and with reduced densities near the critical point, $0.5 \leq \bar{\rho} \leq 1.5$.

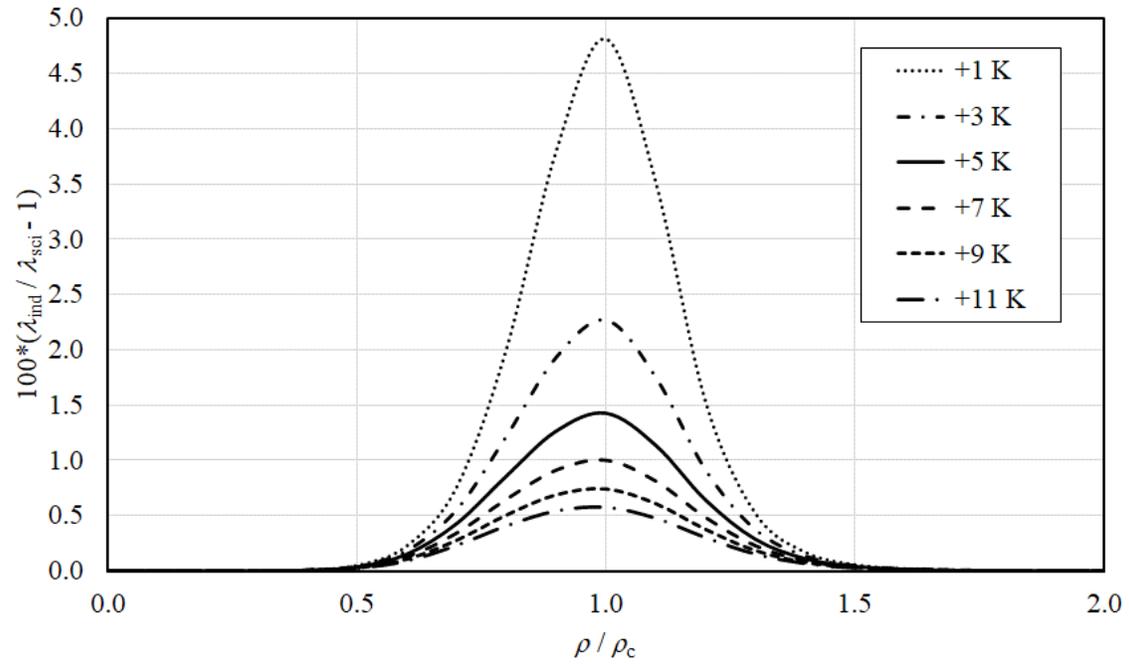


Figure 3. Errors in industrial thermal-conductivity formulation along isotherms near the critical temperature.

3.3. Computer-program verification of industrial equation

Table 6 is provided to assist the user in computer-program verification for industrial use.

Table 6. Sample points for computer-program verification of the correlating equation, Eq. (25), for thermal conductivity (industrial use), including the critical-enhancement contribution $\bar{\lambda}_{21}$. For all points, $\bar{\lambda}_0(644.10 \text{ K}) = 52.149\ 66$ and $T = 644.10 \text{ K}$.

ρ (kg m ⁻³)	$\bar{\lambda}_1$	$\bar{\lambda}_{21}$	λ_1 (mW m ⁻¹ K ⁻¹)
1	1.005 807 6	0.000 120 7	52.4527
106	1.791 564 9	9.912 548 0	103.342
256	3.390 704 3	222.078 865	398.903
306	3.963 958 7	631.959 374	838.678
356	4.518 682 1	1158.467 33	1394.115
406	5.041 459 0	435.258 942	698.169
456	5.529 512 3	138.464 122	426.826
750	8.598 246 1	6.449 056 0	454.845

4. References

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