

Thermophysical properties of sulphur hexafluoride

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THERMOPHYSICAL PROPERTIES OF SULPHUR HEXAFLUORIDE

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THERMOPHYSICAL PROPERTIES OF SULPHUR HEXAFLUORIDE

1. INTRODUCTION

This Item, which is one of a series concerned with the thermophysical properties of industrially important fluids, presents values of the thermophysical properties of sulphur hexafluoride on the saturation line, and in the ideal gas state, the dilute gas state, the gas phase and the supercritical region.

The recommended values of the transport properties are based on data which are considered to be the best available; the recommended values for the thermodynamic properties are derived from the Equation of State in Derivation 27. Along the saturation line the temperature range covered for all properties is from the triple point to within at least 10 kelvin of the critical temperature,. The properties of the ideal and dilute gas are given for temperatures from 222.65 K to 1000 K and the thermodynamic properties of the gas phase and supercritical regions for temperatures from -50 to 100 °C and for pressures up to 10 MPa.

All quantities are expressed in SI units or their multiples (see Section 2) but, for users who require them in other units, conversion factors are provided in Appendix A. Equations representing the saturation properties and those of the ideal and dilute gas are given in Section 3.2, and Section 3.3 gives an explanation of Tables 6.2 to 6.5. The single phase thermodynamic properties are discussed in Section 4. Section 4.1 describes the development of the Helmholtz equation of state and lists the data used to obtain the fundamental equation. Section 4.2 gives an explanation of Tables 6.6 to 6.11 and includes a discussion of the estimated uncertainties.

2. NOTATION AND UNITS

b_1, b_2, b_3, b_4, b_5	constants in Equations (3.1) to (3.17)	*
c	specific heat capacity	kJ/kg K
h	specific enthalpy	kJ/kg
M	molecular weight (relative molecular mass)	—
p	pressure	kPa
r	specific gas constant	kJ/kg K
s	specific entropy	kJ/kg K
T	kelvin temperature	K
t	Celsius temperature, $(T - 273.15)$	°C
u	specific internal energy	kJ/kg
V	molar volume	cm ³ /mol
v	specific volume, $v = 1/\rho$	m ³ /kg
Z	compression factor, $pv/(rT)$	—
η	dynamic viscosity	mN s/m ² or $\mu\text{N s/m}^2$

* The constants b are dimensionless except for the following: Equations (3.4) and (3.6), kJ/kg (all); Equations (3.7) and (3.8), kJ/kg K (b_1); Equation (3.9), K (b_3), mN s/m² (b_4); Equation (3.10), $\mu\text{N s/m}^2$ ($\exp(b_1)$); Equations (3.11) and (3.12), mW/m K (b_1 and $\exp(b_1)$ respectively); Equation (3.13), mN/m (b_1); Equation (3.14), kJ/kg K (all); Equation (3.15), kJ/kg (all); Equation (3.16), $\mu\text{N s/m}^2$ (all); Equation (3.17), mW/m K (all).

θ	temperature dependent variable in Equation (3.9)	–
λ	thermal conductivity	mW/m K
ρ	density	kg/m ³
σ	surface tension	mN/m
μ	Joule-Thomson coefficient	K/kPa
μ_T	Isothermal Joule-Thomson coefficient	m ³ /kg
ω	acentric factor	–

State descriptors

(g)	value for gas or saturated vapour
(l)	value for saturated liquid
Δ	denotes property difference between two states

Superscripts

id	denotes ideal gas
(o)	denotes dilute gas

Subscripts

b	value at normal boiling point
c	value at critical point
T	value at constant temperature
p	value at triple point
p	value at constant pressure
r	denotes reduced quantity, <i>e.g.</i> $T_r = T/T_c$
sat	value at saturation (defined in Appendix B, Section B1)
v	value at constant volume
vap	denotes evaporation.

3. PROPERTIES AT SATURATION, IN THE IDEAL GAS STATE AND DILUTE GAS STATE

3.1 Thermophysical Properties

The equations given in Section 3.2 for the thermodynamic properties on the saturation line were fitted to values calculated from the Helmholtz Equation of State (Derivation 27). Equations (3.9) to (3.12) inclusive for the transport properties on the saturation line were fitted to values derived from a computer software package, codename 'LOADER' (Derivation 29), developed by the National Engineering Laboratory. The properties for the ideal and dilute gas were derived from equations representing the selected literature values.

Tables 6.1 to 6.5 are based on the following data sources:

Physical constants	Derivation 27
Vapour pressure	Derivation 27
Density of the saturated liquid	Derivation 27
Density of the saturated vapour	Derivation 27
Specific enthalpy of the saturated liquid	Derivation 27
Specific enthalpy of the saturated vapour	Derivation 27
Latent heat of vaporisation	Derivation 27
Specific heat capacity of the saturated liquid	Derivation 27
Specific heat capacity of the saturated vapour	Derivation 27
Viscosity of the saturated liquid	Derivation 15
Viscosity of the saturated vapour	Derivation 29
Thermal conductivity of the saturated liquid	Derivation 16
Thermal conductivity of the saturated vapour	Derivation 29
Surface tension of the liquid	Derivations 13 , 17 , 18
Specific heat capacity of the ideal gas	Derivation 19
Viscosity of the dilute gas	Derivation 24
Thermal conductivity of the dilute gas	Derivation 26 .

3.2 Equations for Properties

3.2.1 Vapour pressure

Data for the vapour pressure are represented by Equation [\(3.1\)](#).

$$\log_e \left(\frac{p}{p_c} \right) = \frac{1}{T_r} [b_1(1 - T_r) + b_2(1 - T_r)^{3/2} + b_3(1 - T_r)^{5/2} + b_4(1 - T_r)^5]. \quad (3.1)$$

3.2.2 Density of the saturated liquid

Data for the density of the saturated liquid are represented by Equation [\(3.2\)](#).

$$\log_e \left(\frac{\rho(l)}{\rho_c} \right) = b_1(1 - T_r)^{1/3} + b_2(1 - T_r)^{2/3} + b_3(1 - T_r) + b_4(1 - T_r)^{4/3}. \quad (3.2)$$

3.2.3 Density of the saturated vapour

Data for the density of the saturated vapour are represented by Equation [\(3.3\)](#).

$$\log_e \left(\frac{\rho(g)}{\rho_c} \right) = b_1 \left(\frac{1}{T_r} - 1 \right)^{1/3} + b_2 \left(\frac{1}{T_r} - 1 \right)^{2/3} + b_3 \left(\frac{1}{T_r} - 1 \right) + b_4 \left(\frac{1}{T_r} - 1 \right)^{4/3} + b_5 \left(\frac{1}{T_r} - 1 \right)^{5/3}. \quad (3.3)$$

3.2.4 Specific enthalpy of the saturated liquid

Data for the specific enthalpy of the saturated liquid are represented by Equation (3.4).

$$h(l) = b_1 + b_2(1 - T_r)^{1/3} + b_3(1 - T_r)^{2/3} + b_4(1 - T_r) + b_5(1 - T_r)^{4/3}. \quad (3.4)$$

3.2.5 Latent heat of vaporisation (specific enthalpy of vaporisation)

Data for the latent heat of vaporisation are represented by Equation (3.5).

$$\Delta_{\text{vap}} h = h(g) - h(l). \quad (3.5)$$

3.2.6 Specific enthalpy of the saturated vapour

Data for the specific enthalpy of the saturated vapour are represented by Equation (3.6).

$$h(g) = b_1 + b_2(1 - T_r)^{1/3} + b_3(1 - T_r)^{2/3} + b_4(1 - T_r) + b_5(1 - T_r)^{4/3}. \quad (3.6)$$

3.2.7 Isobaric specific heat capacity of the saturated liquid

Data for the isobaric specific heat capacity of the saturated liquid are represented by Equation (3.7).

$$c_p(l) = b_1[1 + b_2(1 - T_r)^{-1} + b_3(1 - T_r) + b_4(1 - T_r)^2 + b_5(1 - T_r)^3]. \quad (3.7)$$

The significance of $c_p(l)$ as a representation of specific heat capacity is fully explained in Appendix B, Section B1.

3.2.8 Isobaric specific heat capacity of the saturated vapour

Data for the isobaric specific heat capacity of the saturated vapour are represented by Equation (3.8).

$$c_p(g) = b_1[1 + b_2(1 - T_r)^{-2/3} + b_3(1 - T_r)^{-1/3} + b_4(1 - T_r)^{1/3} + b_5(1 - T_r)^{2/3}]. \quad (3.8)$$

The significance of $c_p(g)$ as a representation of specific heat capacity is fully explained in Appendix B, Section B1.

3.2.9 Dynamic viscosity of the saturated liquid

Data for the dynamic viscosity of the saturated liquid are represented by Equation (3.9).

$$\eta(l) = b_4 \exp[b_1(\theta - 1)^{1/3} + b_2(\theta - 1)^{4/3}] \quad (3.9)$$

where $\theta = (T_c - b_3)/(T - b_3)$.

3.2.10 Dynamic viscosity of the saturated vapour

Data for the dynamic viscosity of the saturated vapour are represented by Equation (3.10).

$$\log_e \eta(g) = b_1 + b_2 \left(\frac{1}{T_r} - 1 \right)^{1/3} + b_3 \left(\frac{1}{T_r} - 1 \right)^{4/3}. \quad (3.10)$$

3.2.11 Thermal conductivity of the saturated liquid

Data for the thermal conductivity of the saturated liquid are represented by Equation (3.11).

$$\lambda(l) = b_1[1 + b_2(1 - T_r)^{1/3} + b_3(1 - T_r)^{2/3} + b_4(1 - T_r)]. \quad (3.11)$$

3.2.12 Thermal conductivity of the saturated vapour

Data for the thermal conductivity of the saturated vapour are represented by Equation (3.12).

$$\log_e \lambda(g) = b_1 + b_2(1 - T_r)^{-2/3} + b_3(1 - T_r)^{-1/3} + b_4(1 - T_r)^{1/3} + b_5(1 - T_r)^{2/3}. \quad (3.12)$$

3.2.13 Surface tension

Data for surface tension are represented by Equation (3.13).

$$\sigma = b_1(1 - T_r)^{b_2} [1 + b_3(1 - T_r)]. \quad (3.13)$$

3.2.14 Isobaric specific heat capacity of the ideal gas

Data for the isobaric specific heat capacity of the ideal gas are represented by Equation (3.14).

$$c_p^{\text{id}}(g) = b_1 + b_2 T_r^{-1/2} + b_3 T_r^{1/2} + b_4 T_r. \quad (3.14)$$

3.2.15 Specific enthalpy of the ideal gas

Data for the specific enthalpy of the ideal gas are represented by Equation (3.15).

$$h^{\text{id}}(g) = b_1 + b_2 T_r^{1/2} + b_3 T_r + b_4 T_r^{3/2} + b_5 T_r^2. \quad (3.15)$$

(Equations (3.14) and (3.15) are thermodynamically consistent.)

3.2.16 Dynamic viscosity of the dilute gas

Data for the dynamic viscosity of the dilute gas are represented by Equation (3.16).

$$\eta^{(o)}(g) = b_1 + b_2 T_r + b_3 T_r^2 + b_4 T_r^3. \quad (3.16)$$

3.2.17 Thermal conductivity of the dilute gas

Data for the thermal conductivity of the dilute gas are represented by Equation (3.17).

$$\lambda^{(o)}(g) = b_1 + b_2(1 - T_r) + b_3(1 - T_r)^2 + b_4(1 - T_r)^3. \quad (3.17)$$

3.3 Explanation of Tables 6.1 to 6.5

Table 6.1 provides values of the physical constants and constants for use in the equations given in Section 3.2, that represent the fluid properties in the SI units* of the Notation, Section 2. Modern theory requires the isobaric heat capacity, viscosity and thermal conductivity to tend to infinity as the critical point is approached; this theoretical limit has been included where appropriate in Tables 6.2 and 6.3. However, Equations (3.9), (3.10), (3.11) and (3.12) do not conform with theory in this respect; Equations (3.9), (3.10) and (3.11) approach a finite value and Equation (3.12) goes to zero at the critical temperature. Although the remaining equations, Equations (3.1), (3.2), (3.3), (3.4), (3.5), (3.6), (3.7), (3.8) and (3.13), applying on the saturation line extrapolate in a physically realistic manner, users should not extrapolate any of the equations in Section 3.2 outside the temperature limits specified in Table 6.1.

The values derived from the equations applying on the saturation line, Tables 6.2 and 6.3, are presented from the triple point to approximately $T_r = 0.97$, except for Equations (3.4) and (3.13) which terminate at $T_r = 0.98$ and Equations (3.1), (3.2), (3.3) which are valid to the critical temperature. The specific enthalpy values are calculated on the basis that the enthalpy of the ideal gas is zero at 298.15 K.

The specific enthalpies of vaporisation in column 7 of Tables 6.2 and 6.3 were calculated directly from Equation (3.5) with subsequent rounding to the desired number of significant figures. Small differences, usually in the last figure may occur therefore, between these values and those obtained by subtraction of the specific enthalpies in column 5 from those in column 6, since the values generated thereby are the differences between two rounded numbers.

Parentheses are used in all the tables to indicate the values are not directly supported by experimental data. The thermodynamic data derived from the Helmholtz Equation of State are not marked in this way because they were calculated from an equation covering the whole fluid region which had been fitted to critically evaluated data.

Tables 6.4 and 6.5 present values for the ideal and dilute gas from 222.65 to 1000 K.

Deviations from selected experimental data for the vapour pressure are within $\pm 0.3\%$; for the saturated liquid density they are generally within 0.3% but increase to $\approx 1\%$ at T_c , and for the saturated vapour density are within $\pm 0.5\%$.

4. PROPERTIES IN THE SINGLE PHASE REGION

4.1 Thermodynamic Properties

The Helmholtz Equation of State (Derivation 27) represents the Helmholtz energy as a function of density and temperature from which all the thermodynamic properties are obtained by differentiation. Because a single correlating function is used, all the properties calculated from it are thermodynamically consistent. The function describing the Helmholtz energy contains a total of 33 coefficients which were fitted, by a step-wise weighted least-squares technique with a search procedure, to 1,371 critically selected data points: these included ppT measurements, isobaric and isochoric heat capacities, isenthalpic Joule-Thomson coefficient measurements, and calculated values of the vapour pressure and densities of the saturated liquid and vapour. The equation was constrained to give equality of the Gibbs energy across the saturation boundary. A listing of the relevant data sources, and the temperature, pressure and density ranges is given in Table 4.1. A more detailed description of the experimental data and comparisons with the Helmholtz Equation of State are given in Derivation 27.

* Appendix A gives conversion factors to other units.

TABLE 4.1
Data used in the development of the Helmholtz Equation of State.

Source	Year	Number of data points	Pressure range kPa	Temperature range K	Density range kg/m ³
Single phase properties					
<i>pρT</i>					
Mears <i>et al.</i> [11]	1969	22	300–7900	232–523	146–1753
Ulybin and Zherdev [12]	1971	71	700–55 000	233–473	730–1899
Biswas <i>et al.</i> [22]	1984	158	1900–9600	308–333	131–1256
Biswas <i>et al.</i> [22]	1984	105	120–10 500	333	5.8–1285
Mollerup [23]	1985	51	30–1500	260–285	1.5–127
Abbaci and Sengers [25]	1990	290	3700–5800	318–334	526–979
<i>c_v</i>					
Abbaci and Sengers [25]	1990	68	–	–	–
<i>c_p</i>					
Sirota <i>et al.</i> [20]	1979	522	2390–20 000	298–425	–
Bier <i>et al.</i> [21]	1980	34	100–1500	298–473	–
<i>μ_T</i>					
Bier <i>et al.</i> [21]	1980	35	300–1500	298–473	–
<i>μ_T^(o)</i>					
Bier <i>et al.</i> [21]	1980	7	–	298–473	–
Saturation properties					
<i>c_{sat}(l)</i>					
Eucken and Schröder [10]	1938	2	–	225–230	–
<i>c_v(l)</i>					
Anis'kin [14]	1973	6	–	263–313	–

4.2 Explanation of Tables 6.6 to 6.11

Tables 6.6 to 6.11 present single phase fluid values for, respectively, the density, compression factor, enthalpy, entropy, isobaric specific heat capacity and isochoric specific heat capacity, each in the SI unit of the Notation, Section 2. The range covered is for temperatures from –50 to 100 °C for pressures up to 10 000 kPa. These values were calculated from the Helmholtz Equation of State (Derivation 27); the enthalpy is set to zero in the ideal gas at 298.15 K and the entropy is set to zero in the ideal gas at 298.15 K and 100 kPa.

For the ppT values the deviations of the density from selected experimental data are within $\pm 0.3\%$ for the whole range excluding the critical region. Close to the critical point where the slope of the isotherm $(\partial p / \partial \rho)_T$ is very small the deviation of the densities from the selected values may be large, but deviations of the pressure from the selected values are within $\pm 0.12\%$.

In Tables 6.6 to 6.11 in the neighbourhood of the critical region, there is no method of interpolation which can be relied upon to give accurate results. Therefore all interpolations inside the rectangle formed by the 50 to 60 °C isotherms and the 3500 to 4500 kPa isobars should be regarded as approximations.

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Derivation

The Derivation lists selected sources that have assisted in the preparation of this Data Item.

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