Thermodynamic properties of isopropyl vapor and liquid

All of the liquid and vapor properties and the required correlation for isopropyl alcohol are summarized below.

Viscosity:

The temperature dependence of the viscosity of the gaseous isopropyl may be obtained by the method of corresponding states. From the VDI-Wärmeatlas Blatt Da 25, one obtains the following equation for the viscosity in [Pa s]:

$$\mu = \left[(\mu\ \xi)^{r}\ f_{p} \right] \frac{1}{\xi}$$

With the normalized temperature $T_r = T/T_{crit}$ (T_{crit} is the critical temperature given at the end of this section), one obtains:

$$(\mu\ \xi)^{r} = 0.807\ T_{r} - 0.357\ \exp(-0.449\ T_{r}) + 0.34\ \exp(-4.058\ T_{r}) + 0.018$$

and the factor ξ is calculated from:

$$\xi = \frac{[T_c / K]^{1/6}\ [R/(J/kmolK)]^{1/6}\ [N_A/(1/kmol)]^{1/3}}{[M/(kg/kmol)]^{1/2}\ [p_c/(N/m^2)]^{2/3}}$$

The constant f_p which has to be considered for polar gases is $f_p = 1.141824$ for isopropyl.

Special heat capacity:

The specific heat capacity [kJ/(kg K)] of isopropyl vapor is calculated according to the ideal gas assumption (VDI Wärmeatlas, Blatt Da 21) with the equation:

$$c_{p}^{id} = \frac{4.1868}{M} \left[\sum_{i} n_{i} A_{i} + \sum_{i} n_{i} B_{i} T + \sum_{i} C_{i} T^{2} + \sum_{i} n_{i} D_{i} T^{3} \right]$$

The values of A_i, B_i, C_i and D_i for the individual elements of isopropyl are listed in Table 1.

	A	B	C	D
CH_3	0.6087	2.1433	-0.0852	0.1135
CH	-3.5232	3.4158	-0.2816	0.8015
OH	6.5128	-0.1347	0.0414	-0.1623

Table 1 Constants for CH_3, CH and OH; Isopropyl alcohol: $((CH_3)_2\ CH\ OH)$

For the liquid isopropyl, the heat capacity is obtained by (VDI Wärmeatlas, Blatt Da 23):

$$c_{p,L} = c_p^{id} + \Delta c_p$$

$$\frac{\Delta c_p}{R_m} = 2.56 + 0.436\,(1 - T_r)^{-1} + \omega\left[2.91 + 4.28\,(1 - T_r)^{1/3}\,T_r^{-1} + 0.296\,(1 - T_r)^{-1}\right]$$

with $\omega = 0.669$ and $R_m = R/M$ being the specific gas constant.

The heat capacity of air (mixture of nitrogen and oxygen) was calculated according to Perry (1984):

$$c_{p,air} = 0.79 \cdot c_{p,N2} + 0.21 \cdot c_{p,O2}$$

Thermal conductivity:

For isopropyl alcohol, the thermal conductivity in [kW/(m K)] is calculated from:

$$\lambda = \frac{\mu}{M}\left(1.3\ c_v + 1.843\ R - 1.256\ c_{ir} - \frac{0.347\ R}{T_r} - 3\ \alpha\right)$$

with:

$\alpha = 1.067$

$c_{ir} = 4.38$

$c_v = c_p\, M - R$

The thermal conductivity [W/(m K)] for air is obtained from:

$$\lambda_{air}(T) = \lambda_{air}(373\ K)\,(T/373)^{1.8}$$

with: λ_{air} (373 K) = 0.03139

Vapor pressure:

The vapor pressure for isopropyl is obtained from the Clausius-Clapeyron relation:

$$\ln \frac{p_{s,T}}{p_{s,T_{ref}}} = \frac{\Delta H_v}{R}\left(\frac{1}{T_{ref}} - \frac{1}{T}\right)$$

where ΔH_v is the latent heat of vaporization at temperature T which may be obtained from:

$$\Delta H_v(T) = \Delta H_v(T_{ref}) - \left(\frac{1 - T/T_c}{1 - T_{ref}/T_c}\right)^{0.38}$$

with: ΔH_v (355) = 666.4 kJ/kg (Perry, 1984).

Coefficient of binary diffusion:

The coefficient of binary diffusion for isopropyl in air was measured for different temperatures (e.g. Vargaftik, 1983). The following correlation may be used.

$$D = 4.75\,10^{-10}\ T_{av}^{1.75}\ \left[m^2 / s\right]$$

where T_{av} is the average temperature in the vapor film around the droplet and may be obtained, for example, by the „1/3“ averaging rule.

Additional properties:

Isopropyl:

Molar mass M	60.09	kg/kmol
T_{crit}	508.3	K
P_{crit}	48.2	bar
ρ_1 (liquid)	785	kg/m^3

Air:

Molar mass M	28.84	kg/kmol
T_{crit}	132.5	K
P_{crit}	37.7	bar
ρ (373 K)	0.9329	kg/m^3

References

Perry: Chemical Engineers Handbook, 6th Edition (1984)

Vargaftik: Handbook of Physical Properties of Liquids and Gases, 2 nd Edition (1983)

VDI-Wärmeatlas, VDI-Verlag, 5th Edition (1988)