Hildebrand Solubility Parameter and Mixing Compatibility

Hildebrand solubility parameters of two liquids from their heat of vaporisation and molar volume, and the Flory–Huggins parameter as a compatibility check.

Method: Hildebrand solubility parameter and Flory–Huggins interaction parameter

Input parameters

Unit system: SI

Parameter	Value	Unit
Heat of vaporisation of liquid 1	31.500	kJ/mol
Molar mass of liquid 1	72.150	kg/kmol
Density of liquid 1	626.00	kg/m³
Heat of vaporisation of liquid 2	33.900	kJ/mol
Molar mass of liquid 2	78.110	kg/kmol
Density of liquid 2	876.50	kg/m³
Temperature	25.000	°C

Calculated results

Parameter	Value	Unit
Solubility parameter of liquid 1 (MPa^½)	15.868	
Solubility parameter of liquid 2 (MPa^½)	18.777	
Difference (MPa^½)	2.9092	
Flory–Huggins parameter on the molar volume of liquid 1 (+0.34)	0.73349	

Notes for this case

• The cohesive energy density is the energy to vaporise a unit volume, (ΔH_v − RT)/V_m; its square root is the solubility parameter δ. Liquids with similar δ mix; as a rule of thumb a difference below about 2–4 MPa^½ means miscibility for non-polar liquids. The Flory–Huggins parameter χ = 0.34 + V₁(δ₁ − δ₂)²/RT below about 0.5 indicates a polymer dissolves. Hydrogen-bonding and polar liquids need Hansen's three-part parameters.

Formula and method

$$\delta = \sqrt{\frac{\Delta H_v - RT}{V_m}}, \quad \chi = 0.34 + \frac{V_1(\delta_1 - \delta_2)^2}{RT}$$

Variables

ΔH_{v1}	Heat of vaporisation of liquid 1	J/mol
M_1	Molar mass of liquid 1	kg/kmol
ρ_1	Density of liquid 1	kg/m³
ΔH_{v2}	Heat of vaporisation of liquid 2	J/mol
M_2	Molar mass of liquid 2	kg/kmol
ρ_2	Density of liquid 2	kg/m³
T	Temperature	K
δ_1	Solubility parameter of liquid 1 (MPa^½)	-
δ_2	Solubility parameter of liquid 2 (MPa^½)	-
$\Delta\delta$	Difference (MPa^½)	-
χ	Flory–Huggins parameter on the molar volume of liquid 1 (+0.34)	-

Method and standards

Solubility parameter.

Assumptions and limits

- Regular-solution theory; non-polar liquids.

References

Hildebrand solubility parameter and Flory–Huggins interaction parameter

Report details

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