Wilson Activity Coefficients for a Binary Mixture

Activity coefficients and excess Gibbs energy of a binary liquid by the Wilson equation from user energy parameters and molar volumes, with infinite-dilution values.

Method: Perry's Chemical Engineers' Handbook; 9th ed. (McGraw-Hill, 2019); ...

Input parameters

Unit system: SI

Parameter	Value	Unit
Mole fraction of component 1	30.000	%
Temperature	80.000	°C
Wilson energy a_{12}	399.00	cal/mol
Wilson energy a_{21}	933.00	cal/mol
Molar volume of component 1	58.680	cm³/mol
Molar volume of component 2	18.070	cm³/mol

Calculated results

Parameter	Value	Unit
Activity coefficient of 1	1.6884	
Activity coefficient of 2	1.2072	
γ_1 at infinite dilution	6.6001	
γ_2 at infinite dilution	2.6571	
Excess Gibbs energy / RT	0.28895	

Formula and method

$$\ln\gamma_1 = -\ln(x_1 + \Lambda_{12}x_2) + x_2\left(\frac{\Lambda_{12}}{x_1+\Lambda_{12}x_2} - \frac{\Lambda_{21}}{x_2+\Lambda_{21}x_1}\right)$$

$$\Lambda_{12} = \frac{V_2}{V_1}e^{-a_{12}/RT}, \quad \ln\gamma_1^{\infty} = -\ln\Lambda_{12} + 1 - \Lambda_{21}, \quad \frac{G^E}{RT} = -x_1\ln(x_1+\Lambda_{12}x_2) - x_2\ln(x_2+\Lambda_{21}x_1)$$

Variables

x_1	Mole fraction of component 1	-
T	Temperature	K
a_{12}	Wilson energy a_{12}	J/mol
a_{21}	Wilson energy a_{21}	J/mol
V_1	Molar volume of component 1	m³/mol
V_2	Molar volume of component 2	m³/mol
γ_1	Activity coefficient of 1	-
γ_2	Activity coefficient of 2	-
γ_1^{∞}	γ_1 at infinite dilution	-
γ_2^{∞}	γ_2 at infinite dilution	-
G^E/RT	Excess Gibbs energy / RT	-
R	Gas constant 8.314 462 618	J/(mol·K)

Method and standards

Wilson local-composition model as given in Perry's sec. 4.

Assumptions and limits

- Miscible liquids only.
- The default energies are FireCAD's fit to FireCAD ethanol–water x–y–T data, not published parameters; use literature values for other systems.

References

• Perry's Chemical Engineers' Handbook
• 9th ed. (McGraw-Hill, 2019)
• sec. 4 (thermodynamics: excess Gibbs energy models)
• Wilson equation

Report details

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Results are for engineering estimation. Verify critical designs against the referenced standards and your own data.

This calculator online

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