NRTL Activity Coefficients for a Binary Mixture

Activity coefficients of a binary liquid by the NRTL equation from user parameters b_{12}, b_{21} and non-randomness α, 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
NRTL parameter b_{12} An energy (J/mol or cal/mol). Parameters tabulated in kelvin (b/R) must be multiplied by R = 8.314 J/(mol·K) or 1.987 cal/(mol·K).	478.01	cal/mol
NRTL parameter b_{21} An energy (J/mol or cal/mol). Parameters tabulated in kelvin (b/R) must be multiplied by R = 8.314 J/(mol·K) or 1.987 cal/(mol·K).	956.02	cal/mol
Non-randomness α	0.30000	

Calculated results

Parameter	Value	Unit
Activity coefficient of 1	2.2444	
Activity coefficient of 2	1.2030	
γ_1 at infinite dilution	6.8042	
γ_2 at infinite dilution	4.8862	

Formula and method

$$\ln\gamma_1 = x_2^2\left[\tau_{21}\left(\frac{G_{21}}{x_1+x_2G_{21}}\right)^2+\frac{\tau_{12}G_{12}}{(x_2+x_1G_{12})^2}\right],\quad \tau_{ij}=\frac{b_{ij}}{RT},\quad G_{ij}=e^{-\alpha\tau_{ij}}$$

Variables

x_1	Mole fraction of component 1	-
T	Temperature	K
b_{12}	NRTL parameter b_{12}	J/mol
b_{21}	NRTL parameter b_{21}	J/mol
α	Non-randomness α	-
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	-
$\tau_{12},\tau_{21},G_{12},G_{21}$	NRTL interaction terms	-
R	Gas constant 8.314 462 618	J/(mol·K)

Method and standards

NRTL equation as given in Perry's sec. 4.

Assumptions and limits

- Binary; parameters valid near their fitted temperatures.
- b_{12} and b_{21} are energies (J/mol or cal/mol). Data banks that list them in kelvin (b/R) need them multiplied by R first.

References

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

Report details

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

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