Equilibrium Constant and Conversion from the Gibbs Energy

Equilibrium constant from the standard Gibbs energy of reaction, and the equilibrium conversion for A ⇌ B or a gas-phase A ⇌ 2B at a pressure.

Method: K = exp(−ΔG°/RT) (Smith, Van Ness and Abbott, Introduction to Chemical Engineering Thermodynamics, ch. 13)

Input parameters

Unit system: SI

Parameter	Value	Unit
Standard Gibbs energy of reaction at T	5.0000	kJ/mol
Temperature	326.85	°C
Reaction	A ⇌ B (no mole change)	
Pressure (for A ⇌ 2B)	1.0132	bar
Inert moles per mole of A fed	0	

Calculated results

Parameter	Value	Unit
Equilibrium constant	0.36705	
Equilibrium conversion of A	26.850	%

Notes for this case

- Ideal gas with standard state 1 bar for A ⇌ 2B; ideal solution for A ⇌ B. Raising pressure lowers the conversion of mole-increasing reactions; inerts raise it.

Formula and method

$$K = \exp\left(-\frac{\Delta G^\circ}{RT}\right), \quad X_e = \frac{K}{1+K}\ (A \rightleftharpoons B), \quad K = \frac{(2X/n_T)^2}{(1-X)/n_T}\frac{p}{p^\circ}\ (A \rightleftharpoons 2B)$$

Variables

ΔG°	Standard Gibbs energy of reaction at T	J/mol
T	Temperature	K
type	Reaction	-
p	Pressure (for A ⇌ 2B)	Pa
n_I	Inert moles per mole of A fed	-
K	Equilibrium constant	-
X_e	Equilibrium conversion of A	-

Method and standards

Chemical equilibrium.

Assumptions and limits

- Ideal gas or ideal solution.
- Only two stoichiometries are covered, A ⇌ B and A ⇌ 2B; ΔG° must be the value at the reaction temperature T (use the van 't Hoff calculator to move it from 298 K). R from CODATA.

References

- K = exp(−ΔG°/RT) (Smith, Van Ness and Abbott, Introduction to Chemical Engineering Thermodynamics, ch. 13)

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

https://calc.firecad.com/chemical/reactors/equilibrium-conversion-gibbs

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.