Fugacity Coefficient by Peng–Robinson or SRK

Fugacity coefficient and fugacity of a pure gas or liquid by the Peng–Robinson or SRK equation of state, with Z, molar volume and density.

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

Input parameters

Unit system: SI

Parameter	Value	Unit
Temperature	80.000	°C
Pressure (absolute)	41.352	bar
Critical temperature	132.50	°C
Critical pressure	112.80	bar
Acentric factor	0.25261	
Molar mass	17.031	kg/kmol
Equation of state	Peng–Robinson	
Phase root	Vapour (largest root)	

Calculated results

Parameter	Value	Unit
Compressibility factor	0.74445	
Molar volume	528.60	cm³/mol
Density	32.219	kg/m³
Fugacity coefficient	0.79489	
Fugacity	32.870	bar
Number of physical roots (Z > B)	3.0000	

Notes for this case

- Vapour and liquid roots both exist; the liquid root has the lower fugacity and is the stable phase. The other root is metastable.

Formula and method

$$Z^3-(1-B)Z^2+(A-3B^2-2B)Z-(AB-B^2-B^3)=0\ \text{(PR)},\quad A=\frac{ap}{R^2T^2},\quad B=\frac{bp}{RT}$$

$$a=0.45724\frac{R^2T_c^2}{p_c}\left[1+\kappa(1-\sqrt{T_r})\right]^2,\quad b=0.07780\frac{RT_c}{p_c},\quad \kappa=0.37464+1.54226\omega-0.26992\omega^2$$

$$\ln\phi=Z-1-\ln(Z-B)-\frac{A}{2\sqrt{2}\,B}\ln\frac{Z+(1+\sqrt{2})B}{Z+(1-\sqrt{2})B}\ \text{(PR)}$$

$$Z^3-Z^2+(A-B-B^2)Z-AB=0,\quad a=0.42748\frac{R^2T_c^2}{p_c}\alpha,\quad b=0.08664\frac{RT_c}{p_c},\quad \kappa=0.480+1.574\omega-0.176\omega^2\ \text{(SRK)}$$

$$\ln\phi=Z-1-\ln(Z-B)-\frac{A}{B}\ln\left(1+\frac{B}{Z}\right)\ \text{(SRK)},\quad f=\phi p$$

Variables

T	Temperature	K

p	Pressure	Pa
T_c	Critical temperature	K
p_c	Critical pressure	Pa
ω	Acentric factor	-
M	Molar mass	kg/kmol
EoS	Equation of state	-
root	Phase root	-
Z	Compressibility factor	-
V	Molar volume	m³/mol
ρ	Density	kg/m³
ϕ	Fugacity coefficient	-
f	Fugacity	Pa
n_r	Number of real roots	-

Method and standards

Cubic equation solved analytically; fugacity coefficient from the standard closed forms.

Assumptions and limits

- Pure component; classical mixing rules not included.
- Only roots with Z > B are physical and counted. When vapour and liquid roots both exist, the chosen root is returned and a note says which phase has the lower fugacity (the stable one).

References

• Perry's Chemical Engineers' Handbook
• 9th ed. (McGraw-Hill, 2019)
• sec. 2
• Eq. (2-70) and Table 2-172 (cubic equations of state) and the ammonia worked example

Report details

Report reference	FCC-BKKE-AZ1P (the same inputs always give the same reference)
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Calculator	Fugacity Coefficient by Peng–Robinson or SRK
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Release checks	4 reference cases of this calculator, computed independently, are checked on every release

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

This calculator online

https://calc.firecad.com/chemical/gas-mixtures/fugacity-coefficient-cubic-eos

Open this case on calc.firecad.com →

Reopens the calculator with the inputs of this report.