

# Propane, 2-nitro-2-nitroso-

**Inchi:** InChI=1S/C3H6N2O3/c1-3(2,4-6)5(7)8/h1-2H3  
**InchiKey:** MYRROMXOABKDLG-UHFFFAOYSA-N  
**Formula:** C3H6N2O3  
**SMILES:** CC(C)(N=O)[N+](=O)[O-]  
**Mol. weight [g/mol]:** 118.09  
**CAS:** 5275-46-7

## Physical Properties

Property code	Value	Unit	Source
hf	-292.95	kJ/mol	Joback Method
hvap	46.66	kJ/mol	Joback Method
ie	9.90 ± 0.10	eV	NIST Webbook
log10ws	-1.96		Crippen Method
logp	0.766		Crippen Method
mcvol	82.100	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	480.05	K	Joback Method
tc	701.58	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5275467&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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