

# Urea, 1,3-bis(2-cyanoethyl)-1-nitroso-

**Inchi:** InChI=1S/C7H9N5O2/c8-3-1-5-10-7(13)12(11-14)6-2-4-9/h1-2,5-6H2,(H,10,13)  
**InchiKey:** UJMHIEGWBATPGL-UHFFFAOYSA-N  
**Formula:** C7H9N5O2  
**SMILES:** N#CCCNC(=O)N(CCC#N)N=O  
**Mol. weight [g/mol]:** 195.18  
**CAS:** 60285-25-8

## Physical Properties

Property code	Value	Unit	Source
hf	-17.82	kJ/mol	Joback Method
hvap	76.45	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	0.507		Crippen Method
mcvol	145.330	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	743.60	K	Joback Method
tc	949.52	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C60285258&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  
**log10ws:** 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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