

# Urea, 1-(2-chloroethyl)-1-nitroso-3-(tetrahydrothiopyran

**Inchi:** InChI=1S/C8H14ClN3O2S/c9-3-4-12(11-14)8(13)10-7-1-5-15-6-2-7/h7H,1-6H2,(H,10,13)  
**InchiKey:** XPJOIOLIBUKQBN-UHFFFAOYSA-N  
**Formula:** C8H14ClN3O2S  
**SMILES:** O=NN(CCCl)C(=O)NC1CCSCC1  
**Mol. weight [g/mol]:** 251.73  
**CAS:** 33022-01-4

## Physical Properties

Property code	Value	Unit	Source
hf	-284.38	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	1.814		Crippen Method
mcpvol	174.390	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
tb	667.13	K	Joback Method
tc	887.94	K	Joback Method

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C33022014&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)

## 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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