

# Urea, 1-(2-chloroethyl)-1-nitroso-3-(tetrahydro-4-thiopyr S,S-dioxide

InChI: InChI=1S/C8H14ClN3O4S/c9-3-4-12(11-14)8(13)10-7-1-5-17(15,16)6-2-7/h7H,1-6H2,(H,)  
InChIKey: MHOURTKZILVYRM-UHFFFAOYSA-N

Formula: C8H14ClN3O4S

SMILES: O=NN(CCCl)C(=O)NC1CCS(=O)(=O)CC1

Mol. weight [g/mol]: 283.73

CAS: 33022-02-5

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -779.60 | kJ/mol | Joback Method  |
| hvap          | 80.17   | kJ/mol | Joback Method  |
| log10ws       | -1.86   |        | Crippen Method |
| logp          | 0.495   |        | Crippen Method |
| mcvol         | 186.130 | ml/mol | McGowan Method |
| pc            | 3763.78 | kPa    | Joback Method  |
| tb            | 646.13  | K      | Joback Method  |
| tc            | 844.46  | K      | Joback Method  |

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C33022025&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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