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/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature