Urea, n-(2-chloroethyl)-n-nitroso-n'-(5-nitrothiazol-2-yl)-

Inchi: InChI=1S/C6H6ClN5O4S/c7-1-2-11(10-14)6(13)9-5-8-3-4(17-5)12(15)16/h3H,1-2H2,(H,8

InchiKey: JUYYKEIJMDGWID-UHFFFAOYSA-N

Formula: C6H6ClN5O4S

SMILES: O=NN(CCCl)C(O)=Nc1ncc([N+](=O)[O-])s1

Mol. weight [g/mol]: 279.66

CAS: 33024-33-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	1.819		Crippen Method
mcvol	165.010	ml/mol	McGowan Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33024338&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume