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

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