

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

Inchi:	InChI=1S/C6H7CIN4O3S/c7-1-2-8-5(12)10-6-9-3-4(15-6)11(13)14/h3H,1-2H2,(H2,8,9,10
InchiKey:	DDSHNCNZUCXDDV-UHFFFAOYSA-N
Formula:	C6H7CIN4O3S
SMILES:	O=C(NCCCI)Nc1ncc([N+](=O)[O-])s1
Mol. weight [g/mol]:	250.66
CAS:	3311-98-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.59		Crippen Method
logp	1.412		Crippen Method
mcvol	153.460	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C3311986&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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