5-CHLORO-2-METHYL-3(2H)-ISOTHIAZOLONE

Other names:	3(2H)-Isothiazolone, 5-chloro-2-methyl- 4-Isothiazolin-3-one, 5-chloro-2-methyl- 5-Chloro-2-methyl-4-isothiazolin-3-one 2,3-Dihydro-2-methyl-3-oxo-5-chloroisothiazole 5-chloro-2-methyl-2H-isothiazol-3-one
Inchi:	InChI=1S/C4H4ClNOS/c1-6-4(7)2-3(5)8-6/h2H,1H3
InchiKey:	DHNRXBZYEKSXIM-UHFFFAOYSA-N
Formula:	C4H4ClNOS
SMILES:	Cn1sc(Cl)cc1=O
Mol. weight [g/mol]:	149.60

Physical Properties

Property code	Value	Unit	Source
logp	1.100		Crippen Method
mcvol	92.200	ml/mol	McGowan Method
rinpol	1226.00		NIST Webbook
rinpol	1226.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26172554&Units=SI

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices