

4-Pyrimidinamine, 6-chloro-2-(methylthio)-

Other names:	Pyrimidine, 4-amino-6-chloro-2-(methylthio)- U 8342 4-Amino-6-Chloro-2-methylthiopyrimidine 4-Amino-6-chloro-2-methylmercaptopyrimidine 6-Amino-4-chloro-2-methylmercapto pyrimidine 6-chloro-2-methylthiopyrimidin-4-ylamine
Inchi:	InChI=1S/C5H6ClN3S/c1-10-5-8-3(6)2-4(7)9-5/h2H,1H3,(H2,7,8,9)
InchiKey:	ISUXMAHVLFRZQU-UHFFFAOYSA-N
Formula:	C5H6ClN3S
SMILES:	CSc1nc(N)cc(Cl)n1
Mol. weight [g/mol]:	175.64
CAS:	1005-38-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	1.434		Crippen Method
mcvol	116.080	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1005385&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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