5-Amino-4,6-dichloropyrimidine

Other names:	5-Pyrimidinamine, 4,6-dichloro- Pyrimidine, 5-amino-4,6-dichloro- 4,6-Dichloro-5-aminopyrimidine 4,6-Dichloro-5-pyrimidinamine 4,6-Dichloropyrimidin-5-ylamine
Inchi:	InChI=1S/C4H3Cl2N3/c5-3-2(7)4(6)9-1-8-3/h1H,7H2
InchiKey:	NIGDWBHWHVHOAD-UHFFFAOYSA-N
Formula:	C4H3Cl2N3
SMILES:	Nc1c(Cl)ncnc1Cl
Mol. weight [g/mol]:	163.99
CAS:	5413-85-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	1.366		Crippen Method
mcvol	97.880	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5413854&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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