Pyrimidine, 4,5-diamino-6-chloro-

Other names:	6-chloropyrimidine-4,5-diamine
Inchi:	InChI=1S/C4H5ClN4/c5-3-2(6)4(7)9-1-8-3/h1H,6H2,(H2,7,8,9)
InchiKey:	VNSFICAUILKARD-UHFFFAOYSA-N
Formula:	C4H5ClN4
SMILES:	N=c1[nH]cnc(Cl)c1N
Mol. weight [g/mol]:	144.56
CAS:	4316-98-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	-0.357		Crippen Method
mcvol	95.620	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=C4316987&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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