

5-Amino-6-chloro-4-ethylaminopyrimidine

Inchi:	InChI=1S/C6H9ClN4/c1-2-9-6-4(8)5(7)10-3-11-6/h3H,2,8H2,1H3,(H,9,10,11)
InchiKey:	CSCQRGAUEMMNAS-UHFFFAOYSA-N
Formula:	C6H9ClN4
SMILES:	CCNc1ncnc(Cl)c1N
Mol. weight [g/mol]:	172.62
CAS:	98140-03-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.75		Crippen Method
logp	1.144		Crippen Method
mcvol	123.800	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98140035&Units=SI
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

Legend

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

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