

Pyrimidine, 5-amino-4,6-dichloro-2-ethyl-

Inchi:	InChI=1S/C6H7Cl2N3/c1-2-3-10-5(7)4(9)6(8)11-3/h2,9H2,1H3
InchiKey:	IQHHPQSMYVIVOB-UHFFFAOYSA-N
Formula:	C6H7Cl2N3
SMILES:	CCc1nc(Cl)c(N)c(Cl)n1
Mol. weight [g/mol]:	192.05
CAS:	6237-96-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	1.928		Crippen Method
mcvol	126.060	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=C6237963&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/19-338-6/Pyrimidine-5-amino-4-6-dichloro-2-ethyl.pdf>

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