

Pyrimidine, 2-amino-4-chloro-6-(ethylamino)-

Inchi:	InChI=1S/C6H9ClN4/c1-2-9-5-3-4(7)10-6(8)11-5/h3H,2H2,1H3,(H3,8,9,10,11)
InchiKey:	BVMACTVHXCMJBD-UHFFFAOYSA-N
Formula:	C6H9ClN4
SMILES:	CCNc1cc(Cl)nc(N)n1
Mol. weight [g/mol]:	172.62
CAS:	6316-09-2

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C6316092&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/65-551-8/Pyrimidine-2-amino-4-chloro-6-ethylamino.pdf>

Generated by Cheméo on 2024-04-26 08:37:07.258404057 +0000 UTC m=+16409876.178981378.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.