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/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=C6316092&Units=SI

Legend

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