

4,5-Diamino-6-chloro-2-ethylpyrimidine

Inchi:	InChI=1S/C6H9ClN4/c1-2-3-10-5(7)4(8)6(9)11-3/h2,8H2,1H3,(H2,9,10,11)
InchiKey:	ZUVMNDUMWKEJAD-UHFFFAOYSA-N
Formula:	C6H9ClN4
SMILES:	CCc1nc(N)c(N)c(Cl)n1
Mol. weight [g/mol]:	172.62
CAS:	6237-97-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	0.857		Crippen Method
mcvol	123.800	ml/mol	McGowan Method

Sources

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=C6237974&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/62-314-4/4-5-Diamino-6-chloro-2-ethylpyrimidine.pdf>

Generated by Cheméo on 2024-04-23 11:03:29.6773849 +0000 UTC m=+16159458.597962215.

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