Pyrimidine, 2-amino-4-chloro-5-(p-chlorophenylazo)-6-ethylam

Inchi: InChI=1S/C12H12Cl2N6/c1-2-16-11-9(10(14)17-12(15)18-11)20-19-8-5-3-7(13)4-6-8/h3-

InchiKey: XNQJDZTZJFSYQN-FMQUCBEESA-N

Formula: C12H12Cl2N6

SMILES: CCNc1nc(N)nc(Cl)c1N=Nc1ccc(Cl)cc1

Mol. weight [g/mol]: 311.17

CAS: 6316-10-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.48		Crippen Method
logp	4.213		Crippen Method
mcvol	212.480	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=C6316105&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