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

Inchi: InChI=1S/C10H8Cl2N6/c11-5-1-3-6(4-2-5)17-18-7-8(12)15-10(14)16-9(7)13/h1-4H,(H4,1

InchiKey: VZVFZTIOWNQOBV-ISLYRVAYSA-N

Formula: C10H8Cl2N6

SMILES: Nc1nc(N)c(N=Nc2ccc(Cl)cc2)c(Cl)n1

Mol. weight [g/mol]: 283.12

CAS: 5822-69-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	3.363		Crippen Method
mcvol	184.300	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5822695&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume