

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

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

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