

# 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:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5822695&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5822695&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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