

# Pyrimidine, 2-amino-4-(butylamino)-6-chloro-5-[(p-chlorophenyl)azo]

<b>Inchi:</b>	InChI=1S/C14H16Cl2N6/c1-2-3-8-18-13-11(12(16)19-14(17)20-13)22-21-10-6-4-9(15)5-7
<b>InchiKey:</b>	VAKCXRYHWPKWFC-QURGRASLSA-N
<b>Formula:</b>	C14H16Cl2N6
<b>SMILES:</b>	CCCCNc1nc(N)nc(Cl)c1N=Nc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	339.22
<b>CAS:</b>	92298-20-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.31		Crippen Method
logp	4.993		Crippen Method
mvol	240.660	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C92298209&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92298209&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mvol:</b>	McGowan's characteristic volume

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