

# 9H-purine, 6-dimethylamino, 9-benzyl, 2-chloro-

<b>Inchi:</b>	InChI=1S/C14H14ClN5/c1-20(2)13-11-12(18-14(15)19-13)17-10(16-11)8-9-6-4-3-5-7-9/h
<b>InchiKey:</b>	GREGWVJKCGXFGM-UHFFFAOYSA-N
<b>Formula:</b>	C14H14ClN5
<b>SMILES:</b>	CN(C)c1nc(Cl)nc2[nH]c(Cc3ccccc3)nc12
<b>Mol. weight [g/mol]:</b>	287.75

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	2.181		Crippen Method
mcvol	207.580	ml/mol	McGowan Method

## Sources

<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=B6008307&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008307&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

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

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