

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

<b>Inchi:</b>	InChI=1S/C14H12ClN5/c15-14-17-12(19-6-7-19)11-13(18-14)20(9-16-11)8-10-4-2-1-3-5
<b>InchiKey:</b>	NNZIPUWEWYCMBT-UHFFFAOYSA-N
<b>Formula:</b>	C14H12ClN5
<b>SMILES:</b>	Clc1nc(N2CC2)c2ncn(Cc3ccccc3)c2n1
<b>Mol. weight [g/mol]:</b>	285.73
<b>CAS:</b>	92291-23-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.62		Crippen Method
logp	2.348		Crippen Method
mcvol	196.720	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=C92291231&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92291231&amp;Units=SI</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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