

Purine, 6-aziridiny-9-benzyl-8-chloro-

Inchi:	InChI=1S/C14H12ClN5/c15-14-18-11-12(19-6-7-19)16-9-17-13(11)20(14)8-10-4-2-1-3-5
InchiKey:	RJZDHLHTFYBIC-UHFFFAOYSA-N
Formula:	C14H12ClN5
SMILES:	Clc1nc2c(N3CC3)ncnc2n1Cc1cccc1
Mol. weight [g/mol]:	285.73
CAS:	92291-24-2

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C92291242&Units=SI

Legend

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

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