

9H-purine, 2-amino-6-aziridiny-9-benzyl-

Inchi:	InChI=1S/C14H14N6/c15-14-17-12(19-6-7-19)11-13(18-14)20(9-16-11)8-10-4-2-1-3-5-10
InchiKey:	GUUIYCXRIFFCGL-UHFFFAOYSA-N
Formula:	C14H14N6
SMILES:	<chem>N=c1nc2c(ncn2Cc2ccccc2)c(N2CC2)[nH]1</chem>
Mol. weight [g/mol]:	266.30
CAS:	92495-26-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	0.625		Crippen Method
mcvol	194.460	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92495266&Units=SI
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

Legend

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

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