

Hypoxanthine, 2-(1-aziridiny)-9-benzyl-

Inchi:	InChI=1S/C14H13N5O/c20-13-11-12(16-14(17-13)18-6-7-18)19(9-15-11)8-10-4-2-1-3-5-
InchiKey:	GGQAXKDKAATTBW-UHFFFAOYSA-N
Formula:	C14H13N5O
SMILES:	O=c1[nH]c(N2CC2)nc2c1ncn2Cc1ccccc1
Mol. weight [g/mol]:	267.29
CAS:	6311-27-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	0.506		Crippen Method
mcvol	190.350	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6311279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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