

1-Benzyl-2,3,3-trimethyldiaziridine

Other names:	Diaziridine, 2-benzyl-1,3,3-trimethyl-
Inchi:	InChI=1S/C11H16N2/c1-11(2)12(3)13(11)9-10-7-5-4-6-8-10/h4-8H,9H2,1-3H3
InchiKey:	OIGHGLPKKQEWHM-UHFFFAOYSA-N
Formula:	C11H16N2
SMILES:	CN1N(Cc2ccccc2)C1(C)C
Mol. weight [g/mol]:	176.26
CAS:	77671-19-3

Physical Properties

Property code	Value	Unit	Source
ie	8.88	eV	NIST Webbook
log10ws	-2.66		Crippen Method
logp	2.085		Crippen Method
mcvol	151.190	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=C77671193&Units=SI

Legend

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

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