

1,5-Diazobicyclo[3.2.1]octane, 8-indol-3-yl-

Inchi:	InChI=1S/C14H17N3/c1-2-5-13-11(4-1)12(10-15-13)14-16-6-3-7-17(14)9-8-16/h1-2,4-5,1
InchiKey:	ZWNNWWUKARWDMJ-UHFFFAOYSA-N
Formula:	C14H17N3
SMILES:	c1ccc2c(C3N4CCCN3CC4)c[nH]c2c1
Mol. weight [g/mol]:	227.30
CAS:	197571-82-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.86		Crippen Method
logp	1.706		Crippen Method
mcvol	177.420	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=C197571827&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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