3,9-Diazaoctacyclo[9.3.22,10.0.03,9.04,8.05,15.07,1

Other names: 3,9-Diazaoctacyclo[9.3.2
Inchi: InChI=1S/C14H18N2/c1-2-5-6(3-1)12-10-8-4-7-9(10)11(5)15-13(7)14(8)16(12)15/h5-14H
InchiKey: MSQXNFZTYBJIBK-UHFFFAOYSA-N
Formula: C14H18N2
SMILES: C1CC2C(C1)C1C3C4CC5C3C2N2C5C4N12
Mol. weight [g/mol]: 214.31
CAS: 70873-24-4

Physical Properties

Property code	Value	Unit	Source
ie	7.63	eV	NIST Webbook
log10ws	-2.07		Crippen Method
logp	1.333		Crippen Method
mcvol	152.060	ml/mol	McGowan Method

Sources

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=C70873244&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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