

1,3-Diazatricyclo[3.3.1.1^{3,7}]decane

Other names: 1,3-Diazaadamantane
Inchi: InChI=1S/C8H14N2/c1-7-2-9-4-8(1)5-10(3-7)6-9/h7-8H,1-6H2
InchiKey: QQQIDWOQAXJWFO-UHFFFAOYSA-N
Formula: C8H14N2
SMILES: C1C2CN3CC1CN(C2)C3
Mol. weight [g/mol]: 138.21
CAS: 281-29-8

Physical Properties

Property code	Value	Unit	Source
ie	7.75	eV	NIST Webbook
log10ws	-7.14e-03		Crippen Method
logp	0.211		Crippen Method
mcvol	110.960	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C281298&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

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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