

1,3-Diazaadamantane

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

Physical Properties

Property code	Value	Unit	Source
ie	7.66	eV	Cheméo Relay (1.0)
logp	0.211		Crippen Method
mcvol	110.960	ml/mol	McGowan Method
tb	464.55	K	Cheméo Relay (1.0)
tf	543.37	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C281298&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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<https://www.chemeo.com/cid/57-026-0/1-3-Diazaadamantane.pdf>

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