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