

Naphthalen-1,4-imine, 1,2,3,4-tetrahydro-9-methyl-

Other names:	N-Methyl-11-aza-tricyclo(6.2.1.0(2,7))undec-2,4,6,-triene
Inchi:	InChI=1S/C11H13N/c1-12-10-6-7-11(12)9-5-3-2-4-8(9)10/h2-5,10-11H,6-7H2,1H3
InchiKey:	UWNOWNVIUHVGID-UHFFFAOYSA-N
Formula:	C11H13N
SMILES:	CN1C2CCC1c1cccc12
Mol. weight [g/mol]:	159.23
CAS:	55257-99-3

Physical Properties

Property code	Value	Unit	Source
ie	8.33 ± 0.05	eV	NIST Webbook
log10ws	-2.77		Crippen Method
logp	2.508		Crippen Method
mcvol	130.350	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=C55257993&Units=SI

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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