1H-Indole-3-ethanamine, N-methyl-

Other names:	N«omega»-Methyltryptamine
	Indole, 3-(2-(methylamino)ethyl)-
	Dipterine
	3-(2-(Methylamino)ethyl)indole
	Methyltryptamine
	N-Methyltryptamine
	N-Monomethyltryptamine
	2-(1H-Indol-3-yl)-N-methylethanamine
Inchi:	InChI=1S/C11H14N2/c1-12-7-6-9-8-13-11-5-3-2-4-10(9)11/h2-5,8,12-13H,6-7H2,1H3
InchiKey:	NCIKQJBVUNUXLW-UHFFFAOYSA-N
Formula:	C11H14N2
SMILES:	CNCCc1c[nH]c2ccccc12
Mol. weight [g/mol]:	174.24
CAS:	61-49-4

Physical Properties

Property code	Value	Unit	Source
ie	7.60 ± 0.08	eV	NIST Webbook
log10ws	-2.91		Crippen Method
logp	1.448		Crippen Method
mcvol	146.890	ml/mol	McGowan Method
rinpol	1745.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices