N,N-Dimethyltryptamine

Other names:	1H-Indole-3-ethanamine, N,N-dimethyl-
	Indole, 3-[2-(dimethylamino)ethyl]-
	2-(3-Indolyl)ethyldimethylamine
	3-(2-Dimethylaminoethyl)indole
	Dimethyltryptamine
	DMT
	2-(1H-Indol-3-yl)-N,N-dimethylethanamine
	N,N-dimethyl-1H-indole-3-ethylamine
Inchi:	InChI=1S/C12H16N2/c1-14(2)8-7-10-9-13-12-6-4-3-5-11(10)12/h3-6,9,13H,7-8H2,1-2H3
InchiKey:	DMULVCHRPCFFGV-UHFFFAOYSA-N
Formula:	C12H16N2
SMILES:	CN(C)CCc1c[nH]c2ccccc12
Mol. weight [g/mol]:	188.27
CAS:	61-50-7

Physical Properties

Property code	Value	Unit	Source
ie	7.57 ± 0.05	eV	NIST Webbook
ie	7.30	eV	NIST Webbook
log10ws	-2.71		Crippen Method
logp	1.790		Crippen Method
mcvol	160.980	ml/mol	McGowan Method
rinpol	1745.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C61507&Units=SI

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