5-Methyltryptamine

Other names:	1H-Indole-3-ethanamine, 5-methyl
	Indole, 3-(aminoethyl)-5-methyl-
	5-Methyl-3-(aminoethyl)indole
	Tryptamine, 5-methyl
Inchi:	InChI=1S/C11H14N2/c1-8-2-3-11-10(6-8)9(4-5-12)7-13-11/h2-3,6-7,13H,4-5,12H2,1H3
InchiKey:	PYOUAIQXJALPKW-UHFFFAOYSA-N
Formula:	C11H14N2
SMILES:	Cc1ccc2[nH]cc(CCN)c2c1
Mol. weight [g/mol]:	174.24
CAS:	1821-47-2

Physical Properties

Property code	Value	Unit	Source
ie	7.60	eV	NIST Webbook
ie	7.64 ± 0.05	eV	NIST Webbook
log10ws	-3.21		Crippen Method
logp	1.496		Crippen Method
mcvol	146.890	ml/mol	McGowan Method
rinpol	1795.00		NIST Webbook
rinpol	1795.00		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=C1821472&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