1H-Indole-3-ethanamine, 5-methoxy-N,N-dimethyl-

Other names: Bufotenine, O-methyl-
CT 4334
3-(2-Dimethylaminoethyl)-5-methoxyindole
N,N-Dimethyl-5-methoxytryptamine
Indole, 3-[2-(dimethylamino)ethyl]-5-methoxy-
Methoxybufotenin
5-Methoxydimethyltryptamine
5-Methoxy-N,N-dimethyltryptamine
Methylbufotenine
O-Methylbufotenine
Indole, 3-(2-(N,N-dimethylamino)ethyl)-5-methoxy-
MeODMT
3-(2-(N,N-Dimethylamino)ethyl)-5-methoxyindole
NSC 88624
5-methoxy-N,N-dimethyl-1H-indole-3-ethylamine

Inchi: InChI=1S/C13H18N2O/c1-15(2)7-6-10-9-14-13-5-4-11(16-3)8-12(10)13/h4-5,8-9,14H,6-7

InchiKey: ZSTKHSQDNIGFLM-UHFFFAOYSA-N

Formula: C13H18N2O

SMILES: COc1ccc2[nH]cc(CCN(C)C)c2c1

Mol. weight [g/mol]: 218.29

CAS: 1019-45-0

Physical Properties

Property code	Value	Unit	Source
ie	7.61 ± 0.14	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	1.799		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
rinpol	1960.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1019450&Units=SI

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

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