

Bufotenine

Other names:

1H-Indol-5-ol, 3-[2-(dimethylamino)ethyl]-
Indol-5-ol, 3-[2-(dimethylamino)ethyl]-
Bufotenin
Cinobufotenine
Dimethylserotonin
Mappin
Mappine
N,N-Dimethyl-5-hydroxytryptamine
N,N-Dimethylserotonin
3-[«beta»-(Dimethylamino)ethyl]-5-hydroxyindole
3-[2-(Dimethylamino)ethyl]-5-indolol
3-[2-(Dimethylamino)ethyl]indol-5-ol
5-Hydroxy-N,N-dimethyltryptamine
Cohoba
DM5-HT
NSC 89593

Inchi: InChI=1S/C12H16N2O/c1-14(2)6-5-9-8-13-12-4-3-10(15)7-11(9)12/h3-4,7-8,13,15H,5-6H**InchiKey:** VTTONGPRPXSUTJ-UHFFFAOYSA-N**Formula:** C12H16N2O**SMILES:** CN(C)CCc1c[nH]c2ccc(O)cc12**Mol. weight [g/mol]:** 204.27**CAS:** 487-93-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Crippen Method
logp	1.496		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
rinpol	2123.20		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C487934&Units=SI

Legend

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

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