Bufotenin, monoTMS

Inchi: InChI=1S/C15H24N2OSi/c1-17(2)9-8-12-11-16-15-7-6-13(10-14(12)15)18-19(3,4)5/h6-7,
InchiKey: XXUYWQAQGMCDRE-UHFFFAOYSA-N
Formula: C15H24N2OSi
SMILES: CN(C)CCc1c[nH]c2ccc(O[Si](C)(C)C)cc12
Mol. weight [g/mol]: 276.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	3.004		Crippen Method
rinpol	2090.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R293822&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices