Bufotenin, TMS

Other names: Bufotenin, diTMS
Inchi: InChI=1S/C18H32N2OSi2/c1-19(2)12-11-15-14-20(22(3,4)5)18-10-9-16(13-17(15)18)21-
InchiKey: INEUSXKRQVKPLU-UHFFFAOYSA-N
Formula: C18H32N2OSi2
SMILES: CN(C)CCc1cn([Si](C)(C)C)c2ccc(O[Si](C)(C)C)cc12
Mol. weight [g/mol]: 348.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.83		Crippen Method
logp	4.642		Crippen Method
rinpol	2128.00		NIST Webbook
rinpol	2120.00		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=R94389&Units=SI

Legend

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