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

Latest version available from:
https://www.chemeo.com/cid/47-008-1/Bufotenin-TMS.pdf
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