

N-Methylserotonin, diTMS

Inchi: InChI=1S/C17H30N2OSi2/c1-18-11-10-14-13-19(21(2,3)4)17-9-8-15(12-16(14)17)20-22
InchiKey: MVCNBQDDVPZNDW-UHFFFAOYSA-N
Formula: C17H30N2OSi2
SMILES: CNCCc1cn([Si](C)(C)C)c2ccc(O[Si](C)(C)C)cc12
Mol. weight [g/mol]: 334.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.03		Crippen Method
logp	4.300		Crippen Method
rinpol	2120.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R293842&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/122-729-7/N-Methylserotonin-diTMS.pdf>

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