

N-Acetyl-5-hydroxytryptamine, trimethylsilyl ether

Other names:	N-acetylserotonin, tms derivative
Inchi:	InChI=1S/C15H22N2O2Si/c1-11(18)16-8-7-12-10-17-15-6-5-13(9-14(12)15)19-20(2,3)4/1
InchiKey:	PFRHDGRDPLLVAJ-UHFFFAOYSA-N
Formula:	C15H22N2O2Si
SMILES:	CC(=O)NCCc1c[nH]c2ccc(O[Si](C)(C)C)cc12
Mol. weight [g/mol]:	290.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	2.578		Crippen Method
rinpol	2516.60		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=U352624&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/119-262-9/N-Acetyl-5-hydroxytryptamine-trimethylsilyl-ether.pdf>

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