

1H-Indole, 1-(trimethylsilyl)-5-[(trimethylsilyl)oxy]-3-[2-[(trime

Other names:	5-Hydroxytryptophol, (3TMS)- 5-Hydroxytryptophol, TMS 5-Hydroxytryptophol, 3tms derivative
Inchi:	InChI=1S/C19H35NO2Si3/c1-23(2,3)20-15-16(12-13-21-24(4,5)6)18-14-17(10-11-19(18)
InchiKey:	COSDZRDOTLJSSW-UHFFFAOYSA-N
Formula:	C19H35NO2Si3
SMILES:	C[Si](C)(C)OCCc1cn([Si](C)(C)C)c2ccc(O[Si](C)(C)C)cc12
Mol. weight [g/mol]:	393.74
CAS:	56114-64-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.18		Crippen Method
logp	5.932		Crippen Method
rinpol	2156.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2156.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56114648&Units=SI

Legend

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

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