Tryptamine, mono-TMS

Inchi:	InChI=1S/C13H22N2Si/c1-16(2,3)15-9-8-11-10-14-13-7-5-4-6-12(11)13/h4-7,11,14-15H,
InchiKey:	JGMDTKGVMMVXDL-UHFFFAOYSA-N
Formula:	C13H22N2Si
SMILES:	C[Si](C)(C)NCCC1CNc2ccccc21
Mol. weight [g/mol]:	234.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.06		Crippen Method
logp	3.010		Crippen Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		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=R4385&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/90-724-8/Tryptamine-mono-TMS.pdf
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