

(.+/-.)-3,4-Methylenedioxyamphetamine, N-trimethylsilyl-

Other names:	3,4-Methylenedioxyamphetamine, tms derivative
Inchi:	InChI=1S/C13H21NO2Si/c1-10(14-17(2,3)4)7-11-5-6-12-13(8-11)16-9-15-12/h5-6,8,10,1
InchiKey:	NWGNRXLVLAGOJN-UHFFFAOYSA-N
Formula:	C13H21NO2Si
SMILES:	CC(Cc1ccc2c(c1)OCO2)N[Si](C)(C)C
Mol. weight [g/mol]:	251.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.51		Crippen Method
logp	2.771		Crippen Method
rinpola	1647.40		NIST Webbook
rinpola	1647.40		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352967&Units=SI

Legend

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

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<https://www.cheméo.com/cid/117-562-8/3-4-Methylenedioxyamphetamine-N-trimethylsilyl.pdf>

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