(.+/-.)-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
rinpol	1647.40		NIST Webbook
rinpol	1647.40		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=U352967&Units=SI

Legend

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