(.+/-.)-N-Hydroxy-3,4-methylenedioxyamphetamine trimethylsilyl ether

Other names: N-hydroxy-3,4-(methylenedioxy)amphetamine, tms derivative

Inchi: InChI=1S/C13H21NO3Si/c1-10(14-17-18(2,3)4)7-11-5-6-12-13(8-11)16-9-15-12/h5-6,8,1

InchiKey: MXAFNSUVVHTUMH-UHFFFAOYSA-N

Formula: C13H21NO3Si

SMILES: CC(Cc1ccc2c(c1)OCO2)NO[Si](C)(C)C

Mol. weight [g/mol]: 267.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.59		Crippen Method
logp	2.702		Crippen Method
rinpol	1740.20		NIST Webbook
rinpol	1740.20		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=U352975&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices