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

Other names: N-hydroxy-3,4-(methylenedioxy)amphetamine, tbdms derivative
Inchi: InChI=1S/C16H27NO3Si/c1-12(17-20-21(5,6)16(2,3)4)9-13-7-8-14-15(10-13)19-11-18-14
InchiKey: UEAOPOYRPFBENF-UHFFFAOYSA-N
Formula: C16H27NO3Si
SMILES: CC(Cc1ccc2c(c1)OCO2)NO[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 309.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	3.873		Crippen Method
rinpol	1971.90		NIST Webbook
rinpol	1971.90		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=U352974&Units=SI

Legend

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