

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

Other names:

N-hydroxy-3,4-(methylenedioxy)amphetamine, tbdms derivative

tert-butyl dimethylsilyl ether

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: UEAPOYRPFBNF-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
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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<https://www.chemeo.com/cid/39-769-6/N-Hydroxy-3-4-methylenedioxyamphetamine-tert-butyl dimethylsilyl ether.pdf>

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