R,S-3',4'-methylenedioxy-«alpha»-pyrrolidinoprop ((dihydro-), TMS

Inchi: InChI=1S/C17H27NO3Si/c1-13(18-9-5-6-10-18)17(21-22(2,3)4)14-7-8-15-16(11-14)20-12

InchiKey: JJTWCUGCOFJWFN-UHFFFAOYSA-N

Formula: C17H27NO3Si

SMILES: CC(C(O[Si](C)(C)C)c1ccc2c(c1)OCO2)N1CCCC1

Mol. weight [g/mol]: 321.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	3.792		Crippen Method
rinpol	1965.00		NIST Webbook
rinpol	1980.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290749&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices