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

Inchi: InChI=1S/C17H27NO3Si/c1-13(18-9-7-11-18)17(19)14-8-9-15(20-2)16(12-14)21-22(3
InchiKey: PTCVLNAYOHVFDA-UHFFFAOYSA-N
Formula: C17H27NO3Si
SMILES: COc1ccc(C(=O)C(C)N2CCCC2)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 321.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	3.576		Crippen Method
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R290729&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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