16«alpha»,17-diOH-fujanoic acid, methyl ester TMS ether

Inchi: InChI=1S/C28H50O7Si2/c1-25(14-11-15-26(2,24(31)33-4)22(25)23(30)32-3)21-13-12-20

InchiKey: PUCYDFPNNSORKS-MUBULWPGSA-N

Formula: C28H50O7Si2

SMILES: COC(=O)C1C(C)(C(=O)OC)CCCC1(C)C1CCC2CC1(C=O)CC2(CO[Si](C)(C)C)O[Si](C)(

Mol. weight [g/mol]: 554.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.17		Crippen Method
logp	5.592		Crippen Method
rinpol	3026.00		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=R151783&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices