allo-Cholanic acid, 3«alpha»,7«beta»-dihydroxy, Me-TMS

Other names: 3«alpha»,7«beta»-Dihydroxy-5«alpha»-cholanic acid, methyl ester, TMS
Inchi: InChI=1S/C31H58O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3
InchiKey: FUVKOFYYHKWFJK-GENDGKSSSA-N
Formula: C31H58O4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3259.00		NIST Webbook
rinpol	3259.00		NIST Webbook
rinpol	3259.00		NIST Webbook
ripol	3694.00		NIST Webbook
ripol	3694.00		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=R533492&Units=SI

Legend

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