allo-Cholanic acid, 7«alpha»,12«beta»-dihydroxy, Me-TMS

Other names: 7«alpha»,12«beta»-Dihydroxy-5«alpha»-cholanic acid, methyl ester, TMS

Inchi: InChI=1S/C31H58O4Si2/c1-21(14-17-28(32)33-4)23-15-16-24-29-25(20-27(31(23,24)3)3

InchiKey: WLOQXQFDQGTWNC-HZNNNNMJSA-N

Formula: C31H58O4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CCCCC4(C)C3CC(O[Si](C)(C)C)C12C

Mol. weight [g/mol]: 550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
ripol	3324.00		NIST Webbook
ripol	3324.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R533734&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

ripol: Polar retention indices