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

Other names: 7«alpha»,12«alpha»-Dihydroxy-5«beta»-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-FYCNSXPWSA-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	3162.00		NIST Webbook
rinpol	3162.00		NIST Webbook
rinpol	3162.00		NIST Webbook
ripol	3789.00		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=R534277&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