Cholanic acid, 3«alpha»,6«alpha»,7«alpha»-trihydroxy, Me-TMS

Other names: 3«alpha»,6«alpha»,7«alpha»-Trihydroxy-5«beta»-cholanic acid, methyl ester, TMS
Inchi: InChI=1S/C34H66O5Si3/c1-23(14-17-29(35)36-4)25-15-16-26-30-27(19-21-33(25,26)2)3
InchiKey: MPBUWUAYSDIDGN-FCDWHEFASA-N
Formula: C34H66O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)C(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(
Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3302.00		NIST Webbook
rinpol	3302.00		NIST Webbook
rinpol	3302.00		NIST Webbook
rinpol	3320.00		NIST Webbook
ripol	3563.00		NIST Webbook
ripol	3563.00		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=R533912&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