5-Cholenoic acid, 3-«beta»,12-«alpha»-dihydroxy, methyl ester, TMS

Other names: 3-«beta»,12-«alpha»-Dihydroxy-5-cholenoic acid, MeTMS

Inchi: InChI=1S/C31H56O4Si2/c1-21(11-16-29(32)33-4)25-14-15-26-24-13-12-22-19-23(34-36(

InchiKey: DCHCBDDKWVQOSX-QPLDZBMISA-N

Formula: C31H56O4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C12

Mol. weight [g/mol]: 548.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	8.205		Crippen Method
rinpol	3234.00		NIST Webbook
rinpol	3234.00		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=R393249&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices