Cholanic acid, 3«alpha»,12«alpha»-dihydroxy, Me-TMS

Other names: 3«alpha»,12«alpha»-Dihydroxy-5«beta»-cholanic acid, methyl ester, TMS
5«beta»-Cholanic acid, 3«alpha»,12«alpha»-bis(trimethylsiloxy)-, methyl ester
Methyl 3,12-bis[(trimethylsilyl)oxy]cholan-24-oate, (3«alpha»,5«beta»,12«alpha»)-
3-«alpha»,12-«alpha»-Dihydroxy-5-«beta»-cholanoic acid, MeTMS
5-«beta»-Cholanoic acid, 3-«alpha»-12-«alpha»-dihydroxy, methyl ester, TMS
Deoxycholic acid, trimethylsilyl ether-methyl ester
Methyl desoxycholate, 2tms derivative

Inchi: InChI=1S/C31H58O4Si2/c1-21(11-16-29(32)33-4)25-14-15-26-24-13-12-22-19-23(34-36(

InchiKey: RDYDEBUPRPMEHW-IQLDZALRSA-N

Formula: C31H58O4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(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	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook
rinpol	3260.00		NIST Webbook
rinpol	3174.00		NIST Webbook
rinpol	3174.00		NIST Webbook
rinpol	3200.00		NIST Webbook
rinpol	3247.00		NIST Webbook
rinpol	3174.00		NIST Webbook
ripol	3598.00		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=C6818413&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