Cholan-24-oic acid, 3,12-bis[(trimethylsilyl)oxy]-, methyl ester, (3«alpha»,5«beta»,12«alpha»)-

Other names: 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-UHFFFAOYSA-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

CAS: 6818-41-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3260.00		NIST Webbook
rinpol	3247.00		NIST Webbook
rinpol	3174.00		NIST Webbook
rinpol	3174.00		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