3-«alpha»,6-«alpha»-Dihydroxy-5-«beta»-cholanoi acid, MeTMS

Other names: 3«alpha»,6«alpha»-Dihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether
5-«beta»-Cholanoic acid, 3-«alpha»-6-«alpha»-dihydroxy, methyl ester, TMS
Hyodeoxycholic acid, trimethyl ether-methyl ester

Inchi: InChI=1S/C31H58O4Si2/c1-21(11-14-29(32)33-4)24-12-13-25-23-20-28(35-37(8,9)10)27

InchiKey: FYDBJLGZNQLQEL-HEEYYOORSA-N

Formula: C31H58O4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3282.00		NIST Webbook
rinpol	3256.00		NIST Webbook
rinpol	3224.00		NIST Webbook
rinpol	3224.00		NIST Webbook
rinpol	3224.00		NIST Webbook
rinpol	3256.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R179538&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices