

3«alpha»,12«beta»-Dihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether

Other names:

3-«alpha»,12-«beta»-Dihydroxy-5-«beta»-cholanoic acid, MeTMS
3«alpha»,12«beta»-Dihydroxy-5«beta»-cholanoic acid, trimethylsilyl ether-methyl ester
5-«beta»-Cholanoic acid, 3-«alpha»-12-«beta»-dihydroxy, methyl ester, TMS

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-ZLUMQFPXSA-N
Formula: C31H58O4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C12O
Mol. weight [g/mol]: 550.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3221.00		NIST Webbook
rinpol	3191.00		NIST Webbook
rinpol	3154.00		NIST Webbook
rinpol	3154.00		NIST Webbook
rinpol	3221.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R182306&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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