3«beta»,7«alpha»-Dihydroxy-5«beta»-cholanoic acid, MeTMS

Other names: Methyl 3-«beta»,7-«alpha»-dihydroxy-5-«beta»-cholanoate, TMS

Inchi: InChI=1S/C31H58O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3

InchiKey: FUVKOFYYHKWFJK-QVGSVIFDSA-N

Formula: C31H58O4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 550.96

CAS: 81445-73-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3190.00		NIST Webbook
rinpol	3190.00		NIST Webbook
rinpol	3190.00		NIST Webbook
rinpol	3155.00		NIST Webbook
ripol	3536.00		NIST Webbook
ripol	3536.00		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=C81445730&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