Homochenodeoxycholic acid, trimethylsilyl ether-methyl ester

Other names: 3«alpha»,7«alpha»-Dihydroxy-5«beta»-homocholanoic acid, MeTMS
Inchi: InChI=1S/C32H60O4Si2/c1-22(12-11-13-29(33)34-4)25-14-15-26-30-27(17-19-32(25,26)
InchiKey: WROBMFNTPPQKLK-YOUSAFFKSA-N
Formula: C32H60O4Si2
SMILES: COC(=O)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12
Mol. weight [g/mol]: 564.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	8.675		Crippen Method
rinpol	3339.00		NIST Webbook
rinpol	3366.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R182524&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