3-«alpha»,7-«alpha»-Dihydroxy-12-keto-5-«beta»-c acid, MeTMS

Other names: 5-«beta»-Cholanoic acid, 3-«alpha»,7-«alpha»-dihydroxy-12-one, methyl ester, TMS

Inchi: InChI=1S/C31H56O5Si2/c1-20(11-14-28(33)34-4)23-12-13-24-29-25(19-27(32)31(23,24)

InchiKey: RMBKMRQJJQQWMM-WCJNXRPNSA-N

Formula: C31H56O5Si2

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(=O)C

Mol. weight [g/mol]: 564.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	7.464		Crippen Method
rinpol	3391.00		NIST Webbook
rinpol	3391.00		NIST Webbook
rinpol	3391.00		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=R393209&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices