1-«beta»,3-«alpha»,12-«alpha»-Trihydroxy-5-«beta» acid, MeTMS

Other names: 5-«beta»-Cholanoic acid, 1-«beta»-3-«alpha»,12-«alpha»-trihydroxy, methyl ester, 3TMS

Inchi: InChI=1S/C34H66O5Si3/c1-23(14-19-32(35)36-4)27-17-18-28-26-16-15-24-20-25(37-40(

InchiKey: XULBSWSPHURKBG-DYXBISBCSA-N

Formula: C34H66O5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CC(O[Si](C)(C)C)C4(C)C3CC(O[Si]

Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3296.00		NIST Webbook
rinpol	3296.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R393096&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