3-«alpha»,6-«alpha»,12-«alpha»-Trihydroxy-5-«be
acid, MeTMS

Other names: 5-«beta»-Cholanoic acid, 3-«alpha»,6-«alpha»,12-«alpha»-trihydroxy, methyl ester, TMS

Inchi: InChI=1S/C34H66O5Si3/c1-23(14-17-32(35)36-4)26-15-16-27-25-21-30(38-41(8,9)10)29

InchiKey: UQGJPQVEFKEVQU-XKDDARQZSA-N

Formula: C34H66O5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(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	3280.00		NIST Webbook
rinpol	3280.00		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=R393185&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices