5-«beta»-Cholanoic acid, 3-«alpha»,4-«beta»,12-«alpha»-trihydroxy, methyl ester, TMS

Other names: 3-«alpha»,4-«beta»,12-«alpha»-Trihydroxy-5-«beta»-cholanoic acid, MeTMS
Inchi: InChI=1S/C34H66O5Si3/c1-23(14-19-31(35)36-4)25-17-18-26-24-15-16-27-32(39-42(11,
InchiKey: HUODHVYTPOSCBY-HHBLUBSASA-N
Formula: C34H66O5Si3
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4C(O[Si](C)(C)C)C(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	3390.00		NIST Webbook
rinpol	3390.00		NIST Webbook
rinpol	3390.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R393150&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices