allo-Cholanic acid, 3«beta»,7«beta»,12«beta»-trihydroxy, Me-TMS

Other names: 3«beta»,7«beta»,12«beta»-Trihydroxy-5«alpha»-cholanic acid, methyl ester, TMS

Inchi: InChI=1S/C34H66O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)3

InchiKey: DQKFOBXAKZGIPX-MKJBNUSTSA-N

Formula: C34H66O5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(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	3429.00		NIST Webbook
rinpol	3429.00		NIST Webbook
ripol	3739.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R533650&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

ripol: Polar retention indices

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