3-«alpha»,6-«alpha»,7-«beta»-Trihydroxy-5-«beta» acid, methyl ester, TMS

Other names: 3«alpha»,6«alpha»,7«beta»-Trihydroxy-5«beta»-cholanoic acid, methyl ester, trimethylsilyl ether
3«alpha»,6«alpha»,7«beta»-Trihydroxy-5«beta»-cholanoic acid, MeTMS
«omega»-Muricholic acid, trimethyl ether-methyl ester

Inchi: InChI=1S/C34H66O5Si3/c1-23(14-17-29(35)36-4)25-15-16-26-30-27(19-21-33(25,26)2)3

InchiKey: MPBUWUAYSDIDGN-CQAQCTJOSA-N

Formula: C34H66O5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)C(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4(

Mol. weight [g/mol]: 639.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	9.115		Crippen Method
rinpol	3483.00		NIST Webbook
rinpol	3453.00		NIST Webbook
rinpol	3428.00		NIST Webbook
rinpol	3453.00		NIST Webbook
rinpol	3428.00		NIST Webbook
rinpol	3453.00		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=R182282&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices