3«alpha»,6«beta»,7«beta»-Trihydroxy-5«beta»-ch
acid, MeTMS

Other names: 3«alpha»,6«beta»,7«beta»-Trihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether
3-«alpha»,6-«beta»,7-«beta»-Trihydroxy-5-«beta»-cholic acid, methyl ester, TMS
«beta»-Muricholic acid, trimethyl ether-methyl ester
5-«beta»-Cholanoic acid, 3-«alpha»,6-«beta»,7-«beta»-trihydroxy, methyl ester, TMS
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-ILZJCXJKSA-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	3348.00		NIST Webbook
rinpol	3374.00		NIST Webbook
rinpol	3348.00		NIST Webbook
rinpol	3321.00		NIST Webbook
rinpol	3348.00		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=R182222&Units=SI

Legend

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