3«alpha»,7«alpha»,12«alpha»-Trihydroxy-5«beta»-homocholanoic acid, MeTMS

Other names: Homocholic acid, trimethylsilyl ether-methyl ester
Inchi: InChI=1S/C35H68O5Si3/c1-24(15-14-16-32(36)37-4)27-17-18-28-33-29(23-31(35(27,28)
InchiKey: ATLPMJCJNAJKBU-WEFHNKALSA-N
Formula: C35H68O5Si3
SMILES: COC(=O)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[S
Mol. weight [g/mol]: 653.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	9.505		Crippen Method
rinpol	3350.00		NIST Webbook
rinpol	3384.00		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=R182544&Units=SI

Legend

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