3-oxy-4,6-cholenoate, methyl ester-trimethylsilyl ether

Inchi: InChI=1S/C28H44O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6)

InchiKey: MZSMDUVOYGRVSX-BEVKLEDXSA-N

Formula: C28H44O3Si

SMILES: COC(=O)CCC(C)C1CCC2C3C=CC4=CC(O[Si](C)(C)C)=CCC4(C)C3CCC12C

Mol. weight [g/mol]: 456.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	7.276		Crippen Method

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=R493839&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient