7-Oxo-3«alpha»-hydroxy-5«beta»-cholanic acid, methyl ester, TMS

Inchi: InChI=1S/C28H48O4Si/c1-18(8-11-25(30)31-4)21-9-10-22-26-23(13-15-28(21,22)3)27(2)

InchiKey: FYICTKZKCGJHMG-AUZXRYKPSA-N

Formula: C28H48O4Si

SMILES: COC(=O)CCC(C)C1CCC2C3C(=O)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 476.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.58		Crippen Method
logp	6.634		Crippen Method
rinpol	3315.00		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=R535601&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices