allo-Cholanic acid, 3«beta»-hydroxy, Me-TMS

Other names: 3«beta»-Hydroxy-5«alpha»-cholanic acid, methyl ester, TMS
Inchi: InChI=1S/C28H50O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6)
InchiKey: MMCLGKIAEUXBCF-KSFASEAZSA-N
Formula: C28H50O3Si
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 462.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	7.455		Crippen Method
rinpol	3232.00		NIST Webbook
rinpol	3232.00		NIST Webbook
rinpol	3232.00		NIST Webbook
ripol	3810.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R533690&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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