allo-Cholanic acid, 3«alpha»,7«alpha»-dihydroxy, Me-DMES

Inchi: InChI=1S/C33H62O4Si2/c1-11-38(7,8)36-25-17-19-32(4)24(21-25)22-29(37-39(9,10)12-2

InchiKey: HBVFSTTUJXVCFB-HIYURXDQSA-N

Formula: C33H62O4Si2

SMILES: CC[Si](C)(C)OC1CCC2(C)C(C1)CC(O[Si](C)(C)CC)C1C2CCC2(C)C(C(C)CCC(=O)OC)C

Mol. weight [g/mol]: 579.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	9.065		Crippen Method
rinpol	3429.00		NIST Webbook
rinpol	3429.00		NIST Webbook
ripol	3771.00		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=R533427&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

ripol: Polar retention indices