allo-Cholanic acid, 12«alpha»-hydroxy, Me-DMES

Inchi: InChI=1S/C29H52O3Si/c1-8-33(6,7)32-26-19-25-22(14-13-21-11-9-10-18-28(21,25)3)24-

InchiKey: DBDZGEARTPZCLG-GQPOEMMZSA-N

Formula: C29H52O3Si

SMILES: CC[Si](C)(C)OC1CC2C(CCC3CCCCC32C)C2CCC(C(C)CCC(=O)OC)C12C

Mol. weight [g/mol]: 476.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.72		Crippen Method
logp	7.845		Crippen Method
rinpol	3118.00		NIST Webbook
ripol	3580.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R533269&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