3«alpha»,12«alpha»-dihydroxy-5«beta»-cholan-24 acid, DMESI

Inchi: InChI=1S/C36H70O4Si3/c1-13-41(7,8)38-28-22-23-35(5)27(24-28)17-18-29-31-20-19-30

InchiKey: RIWORMFFYCJZMM-AYROHMKFSA-N

Formula: C36H70O4Si3

SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)CC)CCC4(C)C3CC(O[Si](C

Mol. weight [g/mol]: 651.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	10.660		Crippen Method
rinpol	3410.00		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=R279722&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices