3«alpha»,7«alpha»-dihydroxy-5«beta»-cholan-24-oic acid, DMESI

Inchi: InChI=1S/C36H70O4Si3/c1-13-41(7,8)38-28-20-22-35(5)27(24-28)25-32(39-42(9,10)14-2
InchiKey: NMSWWFYXIZYFHL-JKBYRMPASA-N
Formula: C36H70O4Si3
SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)CC)CC4CC(O[Si](C)(C)CC)CCC4(
Mol. weight [g/mol]: 651.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	10.660		Crippen Method
rinpol	3449.00		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=R279900&Units=SI

Legend

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

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