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

Inchi: InChI=1S/C36H70O4Si3/c1-13-41(7,8)38-28-20-24-35(6)32-22-23-34(5)30(27(4)16-19-3

InchiKey: GUNUQSBFHLXXIW-NFAUZLDOSA-N

Formula: C36H70O4Si3

SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1CCC2C3CCC4(O[Si](C)(C)CC)CC(O[Si](C)(C)CC)CCC4(

Mol. weight [g/mol]: 651.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.19		Crippen Method
logp	10.804		Crippen Method
rinpol	3467.00		NIST Webbook
rinpol	3467.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R279846&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

Latest version available from:

https://www.chemeo.com/cid/53-458-5/3-alpha-5-beta-dihydroxy-5-beta-cholan-24-oic-acid-DMESI.pdf

Generated by Cheméo on 2024-04-23 14:13:25.863103834 +0000 UTC m=+16170854.783681146.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.