3«alpha»,5«beta»,7«beta»-trihydroxy-5«beta»-cho
acid, DMESI

Inchi: InChI=1S/C40H80O5Si4/c1-16-46(8,9)42-31-24-27-39(7)34-25-26-38(6)32(30(5)20-23-3

InchiKey: JQYSIUTVAXNGBU-XWEMHBRLSA-N

Formula: C40H80O5Si4

SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)CC)CC4(O[Si](C)(C)CC)CC(O[Si](

Mol. weight [g/mol]: 753.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	12.024		Crippen Method
rinpol	3610.00		NIST Webbook
rinpol	3610.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R279826&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