3«alpha»,7«beta»,17«alpha»-trihydroxy-5«beta»-c acid, DMESI

Inchi: InChI=1S/C40H80O5Si4/c1-16-46(8,9)42-32-22-25-38(6)31(28-32)29-35(43-47(10,11)17
InchiKey: OBJAMDYRFFJLHC-GAFRAGQESA-N
Formula: C40H80O5Si4
SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1(O[Si](C)(C)CC)CCC2C3C(O[Si](C)(C)CC)CC4CC(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	3620.00		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=R279940&Units=SI

Legend

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