

3«alpha»,7«beta»,14«alpha»-trihydroxy-5«beta»-cholanic 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)17-19)44-20-21-23-24-33-34-36-37-39-40/s1-40/t1-40/m1

InChIKey: VZDYXHOSEUCGAI-YNCWQSMDSA-N

Formula: C₄₀H₈₀O₅Si₄

SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1CCC2(O[Si](C)(C)CC)C3C(O[Si](C)(C)CC)CC4CC(O[Si](C)(C)CC)C14

Mol. weight [g/mol]: 753.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	12.024		Crippen Method
rinpol	3392.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279920&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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