Cholanic acid, 3«alpha»,7«alpha»,12«beta»-trihydroxy, Me-DMES

Inchi: InChI=1S/C37H72O5Si3/c1-14-43(8,9)40-28-21-22-36(5)27(23-28)24-32(41-44(10,11)15

InchiKey: QIHGNFRQNAWOFU-HYGVULDJSA-N

Formula: C37H72O5Si3

SMILES: CC[Si](C)(C)OC1CCC2(C)C(C1)CC(O[Si](C)(C)CC)C1C2CC(O[Si](C)(C)CC)C2(C)C(C(

Mol. weight [g/mol]: 681.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	10.285		Crippen Method
rinpol	3512.00		NIST Webbook
rinpol	3512.00		NIST Webbook
ripol	3729.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R533967&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

ripol: Polar retention indices

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