

3«alpha»,5«beta»,7«alpha»-trihydroxy-5«beta»-cholan-24-oic 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)20-23-31)43-44-45-47-48-49-50-51-52-53-54/s1-16-46(8,9)42-31-24-27-39(7)34-25-26-38(6)32(30(5)20-23-31)43-44-45-47-48-49-50-51-52-53-54/t1-16-46(8,9)42-31-24-27-39(7)34-25-26-38(6)32(30(5)20-23-31)43-44-45-47-48-49-50-51-52-53-54/m1
InChIKey: JQYSIUTVAXNGBU-PTGDQXGESA-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](C)(C)CC)CC5(O[Si](C)(C)CC)CC6(O[Si](C)(C)CC)CC7(O[Si](C)(C)CC)CC8(O[Si](C)(C)CC)CC9(O[Si](C)(C)CC)CC10(O[Si](C)(C)CC)CC11(O[Si](C)(C)CC)CC12(O[Si](C)(C)CC)CC13(O[Si](C)(C)CC)CC14(O[Si](C)(C)CC)CC15(O[Si](C)(C)CC)CC16(O[Si](C)(C)CC)CC17(O[Si](C)(C)CC)CC18(O[Si](C)(C)CC)CC19(O[Si](C)(C)CC)CC20(O[Si](C)(C)CC)CC21(O[Si](C)(C)CC)CC22(O[Si](C)(C)CC)CC23(O[Si](C)(C)CC)CC24(O[Si](C)(C)CC)CC25(O[Si](C)(C)CC)CC26(O[Si](C)(C)CC)CC27(O[Si](C)(C)CC)CC28(O[Si](C)(C)CC)CC29(O[Si](C)(C)CC)CC30(O[Si](C)(C)CC)CC31(O[Si](C)(C)CC)CC32(O[Si](C)(C)CC)CC33(O[Si](C)(C)CC)CC34(O[Si](C)(C)CC)CC35(O[Si](C)(C)CC)CC36(O[Si](C)(C)CC)CC37(O[Si](C)(C)CC)CC38(O[Si](C)(C)CC)CC39(O[Si](C)(C)CC)CC40(O[Si](C)(C)CC)CC

Mol. weight [g/mol]: 753.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	12.024		Crippen Method
rinpol	3582.00		NIST Webbook
rinpol	3582.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279806&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/53-090-3/3-alpha-5-beta-7-alpha-trihydroxy-5-beta-cholan-24-oic-acid-DMESI.pdf>

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