3«alpha»,5«beta»,7«alpha»,17«alpha»-tetrahydroxy-5«beta»-cholan-24-oic acid, DMESI

Inchi: InChI=1S/C44H90O6Si5/c1-19-51(9,10)46-35-26-29-41(7)36-27-30-42(8)37(40(36)38(47

InchiKey: GEAFGDMZJBOVCX-LBRWRNAUSA-N

Formula: C44H90O6Si5

SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1(O[Si](C)(C)CC)CCC2C3C(O[Si](C)(C)CC)CC4(O[Si](C)(

Mol. weight [g/mol]: 855.61

Physical Properties

Property code	Value	Unit	Source
logp	13.389		Crippen Method
rinpol	3733.00		NIST Webbook
rinpol	3733.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R501698&Units=SI

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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