

3«alpha»,7«alpha»,12«alpha»-trihydroxy-5«beta»-bile acid, methyl ester, TMS

InChI: COC(=O)CCC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3C
InChIKey: VDYGYWATAFXFXJX-HNODWYMFSA-N
Formula: C40H76O7Si3
SMILES: COC(=O)CCC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]: 753.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	10.074		Crippen Method
rinpol	3930.00		NIST Webbook
rinpol	3930.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R534920&Units=SI>

Legend

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

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