

24-Hydroxy-trihydroxycoprostanic acid, Me-TMS, isomer 1

Inchi: InChI=1S/C41H82O6Si4/c1-28(2)23-31(45-49(10,11)12)24-29(3)32-19-20-33-37-34(25-30)40-39-38-36-35
InchiKey: AONFNTRSSJNBGS-SHLIRQQNSA-N
Formula: C41H82O6Si4
SMILES: COC(=O)C12CC(O[Si](C)(C)C)CCC1(C)C1CC(O[Si](C)(C)C)C3(C)C(C(C)CC(CC(C)C)O)C3
Mol. weight [g/mol]: 783.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Crippen Method
logp	11.361		Crippen Method
rinpol	3600.00		NIST Webbook
rinpol	3600.00		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=R584886&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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