

3«alpha»,7«alpha»,12«alpha»,24-tetrahydroxy-5«beta»-C27-bile acid, methyl ester, TMS

InChI: InChI=1S/C40H80O6Si4/c1-27(18-21-34(44-48(9,10)11)28(2)38(41)42-5)31-19-20-32-37
InChIKey: OFLKYCRDARMXPS-LNWDKUEZSA-N

Formula: C40H80O6Si4
SMILES: COC(=O)C(C)C(CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]: 769.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.83		Crippen Method
logp	10.971		Crippen Method
rinpol	3600.00		NIST Webbook
rinpol	3612.00		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=R534579&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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