

3«alpha»,6«alpha»,7«alpha»,12«alpha»-tetrahydroxy-5-beta-C27-bile-acid, methyl ester, TMS

Inchi: InChI=1S/C40H80O6Si4/c1-27(19-18-20-28(2)38(41)42-5)30-21-22-31-35-32(26-34(40)39)43-44-45-46/s1-4,19-20,28-29,38-39,41-42,44-45,46-47
InchiKey: SQTBGAFWVHKGDO-QRHLVLFJSA-N
Formula: C40H80O6Si4
SMILES: COC(=O)C(C)CCCC(C)C1CCC2C3C(O[Si](C)(C)C)C(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)C4
Mol. weight [g/mol]: 769.40

Physical Properties

Property code	Value	Unit	Source
logp	10.971		Crippen Method
rinpol	3540.00		NIST Webbook
rinpol	3540.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R534757&Units=SI>

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

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