

3«alpha»,7«alpha»,12«alpha»,25-tetrahydroxy-5«beta»-bile acid, methyl ester, TMS

InChI: InChI=1S/C40H80O6Si4/c1-28(19-18-23-39(3,37(41)42-5)46-50(15,16)17)31-20-21-32-3
InChIKey: ZGBUQCHKVVZJAS-QPRBOIGESA-N
Formula: C40H80O6Si4
SMILES: COC(=O)C(C)(CCCC(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
logp	11.115		Crippen Method
rinpol	3628.00		NIST Webbook
rinpol	3628.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R534886&Units=SI>
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):

Legend

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

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