3«alpha»,7«alpha»,12«alpha»,26-tetrahydroxy-5«b
acid, methyl ester, TMS

Inchi: InChI=1S/C40H80O6Si4/c1-28(18-17-19-29(38(41)42-4)27-43-47(5,6)7)32-20-21-33-37-3
InchiKey: OUCMTBIFLNQXSB-VXIHVOOESA-N
Formula: C40H80O6Si4
SMILES: COC(=O)C(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(
Mol. weight [g/mol]: 769.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Crippen Method
logp	10.973		Crippen Method
rinpol	3715.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R534891&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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