

Cholanoic acid, 3,7-dihydroxy, methyl ester, TMS

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|-----------------------------|--|
| Inchi: | InChI=1S/C31H58O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3 |
| InchiKey: | FUVKOFYYHKWFJK-NNSANRNQSA-N |
| Formula: | C31H58O4Si2 |
| SMILES: | COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12O |
| Mol. weight [g/mol]: | 550.96 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.81 | | Crippen Method |
| logp | 8.285 | | Crippen Method |
| rinpol | 3246.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R394326&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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