

Cholanic acid, 3«beta»,12«alpha»-dihydroxy, Me-TMS

Other names: 3«beta»,12«alpha»-Dihydroxy-5«beta»-cholanic acid, methyl ester, TMS
Inchi: InChI=1S/C31H58O4Si2/c1-21(11-16-29(32)33-4)25-14-15-26-24-13-12-22-19-23(34-36)
InchiKey: RDYDEBUPRPMEHW-BFXJZZGTSA-N
Formula: C31H58O4Si2
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C12C
Mol. weight [g/mol]: 550.96

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.81 | | Crippen Method |
| logp | 8.285 | | Crippen Method |
| rinpola | 3198.00 | | NIST Webbook |
| rinpola | 3198.00 | | NIST Webbook |
| rinpola | 3198.00 | | NIST Webbook |
| ripola | 3545.00 | | NIST Webbook |
| ripola | 3545.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R534099&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/47-023-4/Cholanic-acid-3-beta-12-alpha-dihydroxy-Me-TMS.pdf>

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