# Methyl 7-«alpha»,12«alpha»-dihydroxy-3-keto-4-cholenoa TMS

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|---|---|
| **Other names:** | 7-«alpha»,12-«alpha»-Dihydroxy-3-keto-4-cholenoic acid, MeTMS |
| **Inchi:** | InChI=1S/C31H54O5Si2/c1-20(11-14-28(33)34-4)23-12-13-24-29-25(19-27(31(23,24)3)3 |
| **InchiKey:** | ZMFJVSCTNSUNLT-CGPUBFPPSA-N |
| **Formula:** | C31H54O5Si2 |
| **SMILES:** | COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4=CC(=O)CCC4(C)C3CC(O[Si](C)(C)C) |
| **Mol. weight [g/mol]:** | 562.93 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -3.18 | | Crippen Method |
| logp | 7.384 | | Crippen Method |
| rinpol | 3345.00 | | NIST Webbook |
| rinpol | 3346.00 | | NIST Webbook |

## Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R393581&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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