

3-oxo-4-cholestenoate, O-methyloxime-TMS (2)

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|-----------------------------|--|
| Inchi: | InChI=1S/C31H53NO3Si/c1-21(10-9-11-22(2)29(33)35-36(6,7)8)26-14-15-27-25-13-12-2 |
| InchiKey: | HOMDZWFYFIHOMY-YURFGKIPSA-N |
| Formula: | C31H53NO3Si |
| SMILES: | CON=C1C=C2CCC3C(CCC4(C)C(C(C)CCCC(C)C(=O)O[Si](C)(C)C)CCC34)C2(C)CC1 |
| Mol. weight [g/mol]: | 515.84 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -6.45 | | Crippen Method |
| logp | 8.388 | | Crippen Method |
| rinpol | 3306.00 | | NIST Webbook |
| rinpol | 3306.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R492534&Units=SI |

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/118-858-9/3-oxo-4-cholestenoate-O-methyloxime-TMS-2.pdf>

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