

# Methyl

# 5-«beta»-cholan-7-«alpha»-ol-3-one-24-oate,

Inchi: InChI=1S/C31H57NO4Si2/c1-21(11-14-28(33)34-4)24-12-13-25-29-26(16-18-31(24,25)3  
oxime, TMS # 2  
InchiKey: CQTMZNGJGAEHPX-JRWHHOMKSA-N

Formula: C31H57NO4Si2

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(=NO[Si](C)(C)C)CCC4(C)C3CCC1

Mol. weight [g/mol]: 563.96

## Physical Properties

| Property code | Value   | Unit | Source             |
|---------------|---------|------|--------------------|
| log10ws       | -6.35   |      | Cheméo Relay (1.0) |
| logp          | 8.272   |      | Crippen Method     |
| rinpol        | 3334.00 |      | NIST Webbook       |
| rinpol        | 3334.00 |      | NIST Webbook       |

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R216043&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

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