

# Cholanic acid, 3«alpha»,7«beta»,12«alpha»-trihydroxy, Me-TMS

|                      |  |
|----------------------|--|
| Other names:         | 3«alpha»,7«beta»,12«alpha»-Trihydroxy-5«beta»-cholanic acid, methyl ester, TMS   |
| Inchi:               | InChI=1S/C34H66O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)3 |
| InchiKey:            | DQKFOBXAKZGIPX-ABBGOPQVSA-N  |
| Formula:             | C34H66O5Si3  |
| SMILES:              | COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si]         |
| Mol. weight [g/mol]: | 639.14   |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.31   |      | Crippen Method |
| logp          | 9.115   |      | Crippen Method |
| rinpola       | 3375.00 |      | NIST Webbook   |
| rinpola       | 3375.00 |      | NIST Webbook   |
| rinpola       | 3375.00 |      | NIST Webbook   |

## Sources

|                 |   |
|-----------------|---|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| Crippen Method: | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R534019&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R534019&amp;Units=SI</a> |

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/26-474-7/Cholanic-acid-3-alpha-7-beta-12-alpha-trihydroxy-Me-TMS.pdf>

Generated by Cheméo on 2024-04-26 04:16:34.278295437 +0000 UTC m=+16394243.198872749.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.