

Cholan-24-oic acid, 3,7,12-tris(trimethylsilyl)oxy-, methyl ester, (3«alpha»,5«beta»,7«alpha»12«alpha»)-

Other names:
5«beta»-Cholan-24-oic acid, 3«alpha»,7«alpha»12«alpha»-tris(trimethylsiloxy)-,
Methyl 3,7,12-tris(trimethylsilyl)oxy]cholan-24-oate,
(3«alpha»,5«beta»,7«alpha»12«alpha»)-
3«alpha»,7«alpha»12«alpha»-Trihydroxy-5«beta»-cholanoic acid, methyl
ester-trimethylsilyl ether
3-«alpha»,7-«alpha»12-«alpha»-Trihydroxy-5-«beta»-cholanoic acid, MeTMS
5-«beta»-Cholanoic acid, 3-«alpha»-7-«alpha»12-«alpha»-trihydroxy, methyl
ester, TMS
Cholic acid, methyl ester, TMS
Cholic acid, trimethylsilyl ether-methyl ester
3«alpha»,7«alpha»,12«alpha»-trihydroxy-5«beta»-cholestanoic acid, trimethylsilyl
ether-methyl ester
Methyl cholate, 3tms derivative

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|----------------------|---|
| Inchi: | InChI=1S/C34H66O5Si3/c1-23(14-17-31(35)36-4)26-15-16-27-32-28(22-30(34(26,27)3)35-5-18-29-20-21-22-24-25-26-27-28-29-30-31-32-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-4- |
| InchiKey: | DQKFOBXAKZGIPX-UHFFFAOYSA-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](C)(C)C)C2C |
| Mol. weight [g/mol]: | 639.14 |
| CAS: | 6818-43-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.31 | | Crippen Method |
| logp | 9.115 | | Crippen Method |
| rinpol | 3261.00 | | NIST Webbook |
| rinpol | 3212.00 | | NIST Webbook |
| rinpol | 3212.00 | | 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=C6818435&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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