

Cholan-24-oic acid, 3-[(trimethylsilyl)oxy]-, methyl ester, (3«alpha»,5«beta»)-

Other names:

Methyl 3-[(trimethylsilyl)oxy]cholan-24-oate, (3«alpha»,5«beta»)-
3«alpha»-Hydroxy-5«beta»-cholanoic acid, methyl ester, trimethylsilyl ether
3-«alpha»-Hydroxy-5-«beta»-cholanoic acid, methyl ester, TMS ether
5-«beta»-Cholanoic acid, 3-«alpha».-hydroxy, methyl ester, TMS
Lithocholic acid, trimethylsilyl ether, methyl ester
3«alpha»-hydroxy-5«beta»-cholanoic acid, MeTMS
Methyl lithocholate, (3«alpha»,5«beta»)-, tms derivative

Inchi: InChI=1S/C28H50O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6

InchiKey: MMCLGKIAEUXBCF-UHFFFAOYSA-N

Formula: C28H50O3Si

SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 462.78

CAS: 59953-47-8

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -5.30 | | Crippen Method |
| logp | 7.455 | | Crippen Method |
| rinpol | 3133.00 | | NIST Webbook |
| rinpol | 3179.00 | | NIST Webbook |
| rinpol | 3157.00 | | NIST Webbook |
| rinpol | 3103.00 | | NIST Webbook |
| rinpol | 3103.00 | | NIST Webbook |
| rinpol | 3133.00 | | NIST Webbook |
| ripol | 3647.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C59953478&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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