

«alpha»-Muricholic acid, trimethyl ether-methyl ester

Other names: 3«alpha»,6«beta»,7«alpha»-Trihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether
3«alpha»,6«beta»,7«alpha»-Trihydroxy-5«beta»-cholanoic acid, MeTMS

Inchi: InChI=1S/C34H66O5Si3/c1-23(14-17-29(35)36-4)25-15-16-26-30-27(19-21-33(25,26)2)3

InchiKey: MPBUWUJAYSIDIGN-OCXRKGSLSA-N

Formula: C34H66O5Si3

SMILES: COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)C(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC4

Mol. weight [g/mol]: 639.14

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.31 | | Crippen Method |
| logp | 9.115 | | Crippen Method |
| rinpol | 3246.00 | | NIST Webbook |
| rinpol | 3270.00 | | NIST Webbook |
| rinpol | 3246.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R182202&Units=SI>

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

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

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.cheméo.com/cid/44-981-4/alpha-Muricholic-acid-trimethyl-ether-methyl-ester.pdf>

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