

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

InChI: InChI=1S/C37H72O5Si3/c1-14-43(8,9)40-28-21-22-36(5)27(23-28)24-32(41-44(10,11)15)
InChIKey: QIHGNFRQNAWOFU-QSGQGKPUSA-N
Formula: C37H72O5Si3
SMILES: CC[Si](C)(C)OC1CCC2(C)C(C1)CC(O[Si](C)(C)CC)C1C2CC(O[Si](C)(C)CC)C2(C)C(C(C1)C)C1
Mol. weight [g/mol]: 681.22

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.57 | | Crippen Method |
| logp | 10.285 | | Crippen Method |
| rinpol | 3567.00 | | NIST Webbook |
| ripol | 3868.00 | | 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=R534024&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/69-790-9/Cholanic-acid-3-alpha-7-beta-12-beta-trihydroxy-Me-DMES.pdf>

Generated by Cheméo on 2024-05-03 07:25:19.420502629 +0000 UTC m=+17010368.341079944.

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