

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

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|-----------------------------|--|
| Inchi: | InChI=1S/C33H62O4Si2/c1-11-38(7,8)36-25-19-20-32(4)24(21-25)14-15-26-28-17-16-27 |
| InchiKey: | LNGHMHTXKIMWLA-PUUGMIQCSA-N |
| Formula: | C33H62O4Si2 |
| SMILES: | CC[Si](C)(C)OC1CCC2(C)C(CCC3C2CC(O[Si](C)(C)CC)C2(C)C(C(C)CCC(=O)OC)CCO |
| Mol. weight [g/mol]: | 579.01 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -4.64 | | Crippen Method |
| logp | 9.065 | | Crippen Method |
| rinpol | 3398.00 | | NIST Webbook |
| ripol | 3729.00 | | 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=R534084&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 |

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