

2,3,16,17-Tetrakis(trimethylsilyloxy)estra-1,3,5(16 α ,17 β)-

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|-----------------------------|---|
| Other names: | 2-Hydroxyoestriol, tetrakis-TMS 2-Hydroxyestriol, (4TMS)- 2-Hydroxyoestriol, TMS |
| Inchi: | InChI=1S/C30H56O4Si4/c1-30-17-16-22-23(25(30)20-28(33-37(8,9)10)29(30)34-38(11,12)39)/4-3-5-16-17 |
| InchiKey: | WVBNGTANMJXFH-IUDVKYEMSA-N |
| Formula: | C30H56O4Si4 |
| SMILES: | CC12CCC3c4cc(O[Si](C)(C)C)c(O[Si](C)(C)C)cc4CCC3C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C |
| Mol. weight [g/mol]: | 593.11 |
| CAS: | 51497-46-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.38 | | Crippen Method |
| logp | 9.020 | | Crippen Method |
| rinpol | 3039.00 | | 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=C51497462&Units=SI |

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.chemeo.com/cid/67-973-8/2-3-16-17-Tetrakis-trimethylsilyl-oxy-estra-1-3-5-10-triene-16-alpha-17-beta.p>

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