

16B-Hydroxyoestrone, TMS

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C24H38O3Si2/c1-24-13-12-19-18-11-9-17(26-28(2,3)4)14-16(18)8-10-20(19)2 |
| InchiKey: | OTOYHXDNWUYSAL-UHFFFAOYSA-N |
| Formula: | C24H38O3Si2 |
| SMILES: | CC12CCC3c4ccc(O[Si](C)(C)C)cc4CCC3C1CC(O[Si](C)(C)C)C2=O |
| Mol. weight [g/mol]: | 430.73 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.14 | | Crippen Method |
| logp | 6.155 | | Crippen Method |
| rinpol | 2785.00 | | NIST Webbook |
| rinpol | 2785.00 | | 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=U69368&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/18-912-9/16B-Hydroxyoestrone-TMS.pdf>

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