

1,3,5(10)-Oestratriene-2-methoxy-3,16«alpha»,17«beta»-TMS-16,17-PFP

InChI: COc1cc2c(cc1O[Si](C)(C)C)CCC1C2CCC2(C)C1CC(OC(=O)C(F)(F)C(F)(F)F)C2OC(=O)C(F)(F)C(F)(F)F

InchiKey: SFSIUCCRZYKGTQ-WVFSITQ TSA-N

Formula: C₂₈H₃₂F₁₀O₆Si

SMILES: COc1cc2c(cc1O[Si](C)(C)C)CCC1C2CCC2(C)C1CC(OC(=O)C(F)(F)C(F)(F)F)C2OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 682.62

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -6.89 | | Crippen Method |
| logp | 7.594 | | Crippen Method |
| rinpol | 2747.00 | | NIST Webbook |
| rinpol | 2747.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R537172&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/35-996-8/1-3-5-10-Oestratriene-2-methoxy-3-16-alpha-17-beta-triol-3-TMS-16-17-PFP>.

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