

3,16,17-Trihydroxy-5-abdrosten-11-one, tris-TMS

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|----------------------|---|
| Inchi: | InChI=1S/C28H52O4Si3/c1-27-15-14-20(30-33(3,4)5)16-19(27)12-13-21-22-17-24(31-34) |
| InchiKey: | BYQWGSZSKMWGHT-UHFFFAOYSA-N |
| Formula: | C28H52O4Si3 |
| SMILES: | CC12CCC(O[Si](C)(C)C)CC1=CCC1C2C(=O)CC2(C)C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C |
| Mol. weight [g/mol]: | 536.97 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -0.80 | | Crippen Method |
| logp | 7.398 | | Crippen Method |
| rinpol | 2750.00 | | NIST Webbook |
| rinpol | 2750.00 | | 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=R16563&Units=SI |

Legend

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|----------|-------------------------------------|
| 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/25-827-6/3-16-17-Trihydroxy-5-abdrosten-11-one-tris-TMS.pdf>

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