

3A-Hydroxy-5A-androstan-17-one, enol, bis-TMS

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|-----------------------------|--|
| Inchi: | InChI=1S/C25H46O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27- |
| InchiKey: | WRVSWIFKEWFLRU-PMXONETISA-N |
| Formula: | C25H46O2Si2 |
| SMILES: | CC12CCC3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C |
| Mol. weight [g/mol]: | 434.80 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.15 | | Crippen Method |
| logp | 7.594 | | Crippen Method |
| rinpol | 2536.00 | | NIST Webbook |
| rinpol | 2541.00 | | NIST Webbook |
| rinpol | 2527.00 | | 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=R108724&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/18-412-4/3A-Hydroxy-5A-androstan-17-one-enol-bis-TMS.pdf>

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