

Androsta-1,4-dien-17«beta»-ol-3-one,bis-TMS

Inchi: InChI=1S/C25H42O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey: RUDKDGLQEXQLPE-GECJHHRNSA-N
Formula: C25H42O2Si2
SMILES: CC12C=CC(O[Si](C)(C)C)=CC1=CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 430.77

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.10 | | Crippen Method |
| logp | 7.291 | | Crippen Method |
| rinpol | 2672.00 | | NIST Webbook |
| rinpol | 2685.00 | | NIST Webbook |
| rinpol | 2672.00 | | 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=R319409&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/45-881-4/Androsta-1-4-dien-17-beta-ol-3-one-bis-TMS.pdf>

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