

Etiocholanolone (5B-Androstan-3A-ol-17-one), TMS

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-UFXNSLRTSA-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 |
| rmpol | 2548.00 | | NIST Webbook |
| rmpol | 2548.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R585587&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rmpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/54-522-2/Etiocholanolone-5B-Androstan-3A-ol-17-one-TMS.pdf>

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