

5«alpha»-Androstane-3«alpha»,17«beta»-diol,bis-

Other names: 5-«alpha»-Androstan-3-«alpha»,17-«beta»-diol, TMS
Inchi: InChI=1S/C25H48O2Si2/c1-24-15-13-19(26-28(3,4)5)17-18(24)9-10-20-21-11-12-23(27-
InchiKey: KBSHKNYEUGMMDQ-WGEPUIJFSSA-N
Formula: C25H48O2Si2
SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 436.82

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -2.92 | | Crippen Method |
| logp | 7.469 | | Crippen Method |
| rinpol | 2554.00 | | NIST Webbook |
| rinpol | 2574.00 | | NIST Webbook |
| rinpol | 2575.00 | | NIST Webbook |
| rinpol | 2560.00 | | NIST Webbook |
| rinpol | 2557.00 | | NIST Webbook |
| rinpol | 2535.00 | | NIST Webbook |
| rinpol | 2567.00 | | NIST Webbook |
| rinpol | 2569.00 | | NIST Webbook |
| rinpol | 2567.00 | | NIST Webbook |
| rinpol | 2554.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R319276&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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