

# 5«alpha»-Androstan-3«alpha»-ol-11,17-dione, TMS

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C28H52O3Si3/c1-27-17-16-21(29-32(3,4)5)18-20(27)12-13-22-23-14-15-25(31) |
| InchiKey:            | UYDZAYKIFRXYGS-CVGZZIGOSA-N                                                       |
| Formula:             | C28H52O3Si3                                                                       |
| SMILES:              | CC12C=C(O[Si](C)(C)C)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C           |
| Mol. weight [g/mol]: | 520.97                                                                            |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -1.90   |      | Crippen Method |
| logp          | 8.550   |      | Crippen Method |
| rinpol        | 2647.00 |      | NIST Webbook   |
| rinpol        | 2611.00 |      | NIST Webbook   |
| rinpol        | 2569.00 |      | NIST Webbook   |
| rinpol        | 2647.00 |      | NIST Webbook   |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R321818&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R321818&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method: | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |

## Legend

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

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