

# 5«beta»-Pregnane, 3«alpha»,11«beta»,17,20«alpha»,21-pentakis(trimethylsilyloxy)-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Silane,<br>(5«beta»-pregnane-3«alpha»,11«beta»,17,20«alpha»,21-pentaylpentaoxy)pentakis(trimethylsilyloxy)pregnane,<br>(3«alpha»,5«beta»,11«beta»,20«alpha»)-Cortol, (pentakis-TMS)-<br>A-Cortol, MO TMS<br>A-Cortol, TMS |
| <b>Inchi:</b>               | InChI=1S/C36H76O5Si5/c1-34-22-20-28(38-43(6,7)8)24-27(34)18-19-29-30-21-23-36(41-42)5-6   |
| <b>InchiKey:</b>            | DUBRZSYNDDSLBA-CCWYXXQQA-N  |
| <b>Formula:</b>             | C36H76O5Si5   |
| <b>SMILES:</b>              | CC12CCC(O[Si](C)(C)C)CC1CCC1C2C(O[Si](C)(C)C)CC2(C)C1CCC2(O[Si](C)(C)C)C(C)C1   |
| <b>Mol. weight [g/mol]:</b> | 729.41  |
| <b>CAS:</b>                 | 32213-62-0  |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | 0.84    |      | Crippen Method |
| logp          | 10.741  |      | Crippen Method |
| rinpol        | 3108.00 |      | NIST Webbook   |
| rinpol        | 3150.00 |      | NIST Webbook   |
| rinpol        | 3122.00 |      | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C32213620&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C32213620&amp;Units=SI</a> |

## Legend

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

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