

# 5-«alpha»-Pregnan-3-«alpha»-16-«alpha»,20-«alpha»-triol, MeTMS

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | 5-«alpha»-Pregnan-3-«alpha»,16-«alpha»,20-«alpha»-triol, MeTMS                   |
| Inchi:               | InChI=1S/C30H60O3Si3/c1-21(31-34(4,5)6)28-27(33-36(10,11)12)20-26-24-14-13-22-19 |
| InchiKey:            | GKSDWCMXICLASA-DPVWKVRXSA-N                                                      |
| Formula:             | C30H60O3Si3                                                                      |
| SMILES:              | CC(O[Si](C)(C)C)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C        |
| Mol. weight [g/mol]: | 553.05                                                                           |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.02   |      | Crippen Method |
| logp          | 8.935   |      | Crippen Method |
| rinpol        | 2894.00 |      | NIST Webbook   |
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## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| 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>                         |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R393318&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R393318&amp;Units=SI</a> |

## Legend

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

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