

# METHENOLONE diTMS

|                      |                                                                                           |
|----------------------|-------------------------------------------------------------------------------------------|
| Other names:         | Methenolone (5A-Androst-1-en-1-methyl-17B-ol-3-one), TMS                                  |
| Inchi:               | InChI=1S/C26H46O2Si2/c1-18-16-20(27-29(4,5)6)17-19-10-11-21-22-12-13-24(28-30(7,8)9)25-23 |
| InchiKey:            | UYGZRVZYMDVGDD-UHFFFAOYSA-N                                                               |
| Formula:             | C <sub>26</sub> H <sub>46</sub> O <sub>2</sub> Si <sub>2</sub>                            |
| SMILES:              | CC1=CC(O[Si](C)(C)C)=CC2CCC3C4CCC(O[Si](C)(C)C)C4(C)CCC3C12C                              |
| Mol. weight [g/mol]: | 446.82                                                                                    |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| logp          | 7.761   |      | Crippen Method |
| rinpol        | 2797.00 |      | NIST Webbook   |

## 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>                         |
| Cheméo Relay (1.0):       |                                                                                                                                           |
| Cheméo Relay (1.0, beta): |                                                                                                                                           |
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U331726&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U331726&amp;Units=SI</a> |

## Legend

|         |                                     |
|---------|-------------------------------------|
| logp:   | Octanol/Water partition coefficient |
| rinpol: | Non-polar retention indices         |

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