

# 16«beta»-Hydroxy-dehydroepiandrosterone, MO-TMS

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C26H47NO3Si2/c1-25-14-12-19(29-31(4,5)6)16-18(25)10-11-20-21(25)13-15-2 |
| <b>InchiKey:</b>            | SROWHFXQCWCWEL-ISLFKZSQSA-N  |
| <b>Formula:</b>             | C26H47NO3Si2   |
| <b>SMILES:</b>              | CON=C1C(O[Si](C)(C)C)CC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C                   |
| <b>Mol. weight [g/mol]:</b> | 477.83   |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.67   |      | Crippen Method |
| logp          | 7.002   |      | Crippen Method |
| rinpol        | 2840.00 |      | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R537083&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R537083&amp;Units=SI</a> |
| <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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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<https://www.cheméo.com/cid/47-873-1/16-beta-Hydroxy-dehydroepiandrosterone-MO-TMS.pdf>

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