

# 3«beta»-Hydroxy-5«alpha»-androstane-7,17-dione

**TMS**

**InchiKey:**

InChI=1S/C25H44O3Si2/c1-24-13-11-18(27-29(3,4)5)15-17(24)16-21(26)23-19-9-10-22(

UXGJXQUHLPDPFL-PDQSXKPLSA-N

**Formula:**

C<sub>25</sub>H<sub>44</sub>O<sub>3</sub>Si<sub>2</sub>

**SMILES:**

CC12CCC3C(C(=O)CC4CC(O[Si](C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C

**Mol. weight [g/mol]:**

448.79

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.43		Crippen Method
logp	6.774		Crippen Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook

## Sources

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R307025&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**log10ws:**

Log10 of Water solubility in mol/l

**logp:**

Octanol/Water partition coefficient

**rinpol:**

Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/65-759-8/3-beta-Hydroxy-5-alpha-androstane-7-17-dione-TMS.pdf>

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