

# 3«alpha»,16«beta»,17«alpha»-Trihydroxy-5«beta»

Other names:  
**tris-TMS**

3A,16B,17A-Trihydroxy-5B-androstane, TMS

Inchi: InChI=1S/C28H56O3Si3/c1-27-16-14-21(29-32(3,4)5)18-20(27)12-13-22-23(27)15-17-28

InchiKey: RQCSPBXXGJRUKU-KBNVHCSPSA-N

Formula: C28H56O3Si3

SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C

Mol. weight [g/mol]: 525.00

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	8.299		Crippen Method
rinpol	2747.00		NIST Webbook
rinpol	2648.00		NIST Webbook
rinpol	2747.00		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=R16648&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**rinpol:** Non-polar retention indices

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<https://www.chemeo.com/cid/61-852-8/3-alpha-16-beta-17-alpha-Trihydroxy-5-beta-androstane-tris-TMS.pdf>

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