

# 5-«alpha»-Androstan-3-one, TMS

**Inchi:** InChI=1S/C22H38OSi/c1-21-12-6-7-19(21)18-9-8-16-15-17(23-24(3,4)5)10-14-22(16,2)2  
**InchiKey:** AQAMOROYYHHHDH-ZSFLQZPOSA-N  
**Formula:** C22H38OSi  
**SMILES:** CC12CCCC1C1CCC3CC(O[Si](C)(C)C)=CCC3(C)C1CC2  
**Mol. weight [g/mol]:** 346.62

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	6.764		Crippen Method
rinpol	2195.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2195.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=R149710&Units=SI>

## 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/22-292-3/5-alpha-Androstan-3-one-TMS.pdf>

Generated by Cheméo on 2024-05-01 08:22:59.467105698 +0000 UTC m=+16841028.387683010.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.