

3«alpha»,16«alpha»,17«beta»-Trihydroxy-5«beta»-androstane-tris-TMS

Other names:	5B-Androstan-3A,16A,17B-triol, tris-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-MGLWDPHUSA-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	2752.00		NIST Webbook
rinpol	2753.00		NIST Webbook
rinpol	2752.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R16620&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/44-173-1/3-alpha-16-alpha-17-beta-Trihydroxy-5-beta-androstane-tris-TMS.pdf>

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