

5B-Androstan-3A,16B,17B-triol, tris-TMS

Other names:	3A,16B,17B-Trihydroxy-5B-androstane, tris-TMS 3«alpha»,16«beta»,17«beta»-Trihydroxy-5«beta»-androstane, 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-DEMIQJKMSA-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	2798.00		NIST Webbook
rinpol	2803.00		NIST Webbook
rinpol	2807.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R16652&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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