

3B,16A,17B-Trihydroxyandrost-5-ene, tris-TMS

Other names:	Androst-5-ene-3«beta»,16«alpha»,17«beta»-triol, TMS
Inchi:	InChI=1S/C28H54O3Si3/c1-27-16-14-21(29-32(3,4)5)18-20(27)12-13-22-23(27)15-17-28
InchiKey:	HVNNEDKUOOQWAG-OXKJMOMGSA-N
Formula:	C28H54O3Si3
SMILES:	CC12CCC(O[Si](C)(C)C)CC1=CCC1C2CCC2(C)C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]:	522.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.52		Crippen Method
logp	8.219		Crippen Method
rinpole	2889.00		NIST Webbook
rinpole	2858.00		NIST Webbook
rinpole	2889.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R108759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.cheméo.com/cid/59-329-2/3B-16A-17B-Trihydroxyandrost-5-ene-tris-TMS.pdf>

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