

5B-Androstan-3B,16B,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-SCOJJNELSA-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	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R295353&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/46-851-6/5B-Androstan-3B-16B-17B-triol-tris-TMS.pdf>

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