

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

InChI: InChI=1S/C28H54O4Si3/c1-27-15-14-20(30-33(3,4)5)16-19(27)12-13-21-22-17-24(31-34)3-2
InChIKey: XXWSAVATEUEKOY-XOSHAVBHSA-N
Formula: C28H54O4Si3
SMILES: CC12CC(=O)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CC(O[Si](C)(C)C)C2O[Si](C)(C)C
Mol. weight [g/mol]: 538.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.70		Crippen Method
logp	7.478		Crippen Method
rinpol	2856.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R16602&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

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<https://www.cheméo.com/cid/69-198-7/3-alpha-16-alpha-17-beta-Trihydroxy5-beta-androstan-11-one-tris-TMS.pdf>

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