

5«beta»-Androstan-6«beta»-ol-3,17-dione, tris-TMS

Inchi: InChI=1S/C28H52O3Si3/c1-27-16-14-20(29-32(3,4)5)18-24(27)25(30-33(6,7)8)19-21-22
InchiKey: ZNMLKZDNEJOGCO-QZOMAZOESA-N
Formula: C28H52O3Si3
SMILES: CC12CCC3C(CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)=CCC43C)C1CC=C2O[Si](C)(C)C
Mol. weight [g/mol]: 520.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	8.550		Crippen Method
rinpol	2586.00		NIST Webbook
rinpol	2588.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R319370&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/67-291-5/5-beta-Androstan-6-beta-ol-3-17-dione-tris-TMS.pdf>

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