

3«alpha»,15«alpha»-dihydroxy-5«beta»-androstane-17-one-TMS

InChIKey:

InChI=1S/C28H54O3Si3/c1-27-16-14-21(29-32(3,4)5)18-20(27)12-13-22-23(27)15-17-28
VFJHDKUHDGAWQC-QZFPZXFTSA-N

Formula:

C28H54O3Si3

SMILES:

CC12CCC3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1C(O[Si](C)(C)C)C=C2O[Si](C)(C)C

Mol. weight [g/mol]:

522.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	8.424		Crippen Method
rinpol	2621.00		NIST Webbook
rinpol	2572.00		NIST Webbook
rinpol	2621.00		NIST Webbook

Sources

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R488169&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/54-567-3/3-alpha-15-alpha-dihydroxy-5-beta-androstan-17-one-TMS.pdf>

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