

3«beta»,7«beta»-Dihydroxy-5«alpha»-androstan-17-one-TMS

TMS

InChI=1S/C28H54O3Si3/c1-27-16-14-21(29-32(3,4)5)18-20(27)19-24(30-33(6,7)8)26-22

InchiKey:

VMAJAJNKRDOOQG-QGYZHIDISA-N

Formula:

C28H54O3Si3

SMILES:

CC12CCC3C(C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC43C)C1CC=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	2798.00		NIST Webbook
rinpol	2798.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R307005&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/31-514-6/3-beta-7-beta-Dihydroxy-5-alpha-androstan-17-one-TMS.pdf>

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