

5«beta»-Androstan-3«alpha»,11«beta»-diol-17-one

TMS

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C28H54O3Si3/c1-27-17-16-21(29-32(3,4)5)18-20(27)12-13-22-23-14-15-25(31

HTALMMXGRYNYNV-YTCVGTBISA-N

C28H54O3Si3

CC12CC(O[Si](C)(C)C)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CC=C2O[Si](C)(C)C

522.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	8.424		Crippen Method
rinpola	2696.00		NIST Webbook
rinpola	2672.00		NIST Webbook
rinpola	2696.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R321883&Units=SI>

Crippen Method:

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

Crippen Method:

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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpola: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/42-714-2/5-beta-Androstan-3-alpha-11-beta-diol-17-one-TMS.pdf>

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