

5«alpha»-Androstane-3«alpha»,6«beta»,17«beta»-TMS

TMS

InchiKey:

InChI=1S/C28H56O3Si3/c1-27-16-14-20(29-32(3,4)5)18-24(27)25(30-33(6,7)8)19-21-22

KVQPAVGFDTUVFY-BGDOSBNASA-N

Formula:

C28H56O3Si3

SMILES:

CC12CCC3C(CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)CCC43C)C1CCC2O[Si](C)(C)C

Mol. weight [g/mol]:

525.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	8.299		Crippen Method
rinpol	2697.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R307109&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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.chemeo.com/cid/13-445-3/5-alpha-Androstane-3-alpha-6-beta-17-beta-triol-TMS.pdf>

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