

5«alpha»-Androstane-2«beta»,3«beta»,17«beta»-triol-TMS

TMS

InChI=1S/C28H56O3Si3/c1-27-17-16-23-21(22(27)14-15-26(27)31-34(9,10)11)13-12-20

InchiKey:

AHPKNGPAYNSDOO-WAGGLAFESA-N

Formula:

C₂₈H₅₆O₃Si₃

SMILES:

CC12CC(O[Si](C)(C)C)C(O[Si](C)(C)C)CC1CCC1C2CCC2(C)C(O[Si](C)(C)C)CCC12

Mol. weight [g/mol]:

525.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	8.299		Crippen Method
rinpol	2869.00		NIST Webbook
rinpol	2869.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R307050&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.chemeo.com/cid/63-513-2/5-alpha-Androstane-2-beta-3-beta-17-beta-triol-TMS.pdf>

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