

Oxymesterone (Androst-4-en-17A-methyl-4,17B-diol-3-one), TMS

InChIKey:

InChI=1S/C29H54O3Si3/c1-27-18-17-25(30-33(4,5)6)26(31-34(7,8)9)24(27)14-13-21-22

Formula:

C₂₉H₅₄O₃Si₃

SMILES:

CC12CC=C(O[Si](C)(C)C)C(O[Si](C)(C)C)=C1CCC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C

Mol. weight [g/mol]:

534.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	9.084		Crippen Method
rinpol	2984.00		NIST Webbook
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Sources

Crippen Method:

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

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R585681&Units=SI>

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/62-542-1/Oxymesterone-Androst-4-en-17A-methyl-4-17B-diol-3-one-TMS.pdf>

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