

6«beta»-Hydroxy-17«alpha»-Methyltestosterone, tris-TMS (3,5-diene)

Inchi: C[C@H](O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C(C)C
InchiKey: SOCIYQIICHPHEZ-DEQZDSFDSA-N

Formula: C₂₉H₅₄O₃Si₃

SMILES: CC12CCC(O[Si](C)(C)C)=CC1=C(O[Si](C)(C)C)CC1C2CCC2(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	2905.00		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=R263079&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/47-998-3/6-beta-Hydroxy-17-alpha-Methyltestosterone-tris-TMS-3-5-diene.pdf>

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