

6«alpha»-Hydroxy-Testosterone, tris-TMS (3,5-diene)

Inchi: InChI=1S/C28H52O3Si3/c1-27-16-14-20(29-32(3,4)5)18-24(27)25(30-33(6,7)8)19-21-22
InchiKey: ZANGAJCOGYENPK-VM ECOXCJSA-N
Formula: C₂₈H₅₂O₃Si₃
SMILES: CC12CCC(O[Si](C)(C)C)=CC1=C(O[Si](C)(C)C)CC1C2CCC2(C)C(O[Si](C)(C)C)CCC12
Mol. weight [g/mol]: 520.97

Physical Properties

Property code	Value	Unit	Source
logp	8.694		Crippen Method
rinpol	2823.00		NIST Webbook
rinpol	2823.00		NIST Webbook
rinpol	2823.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R495959&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-960-1/6-alpha-Hydroxy-Testosterone-tris-TMS-3-5-diene.pdf>

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