

6«alpha»-Hydroxy-Testosterone, tris-TMS (2,4-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: QIKQPHVZLFLMDP-JCUQEKLKSA-N
Formula: C28H52O3Si3
SMILES: CC12CC=C(O[Si](C)(C)C)C=C1C(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
log10ws	-1.75		Crippen Method
logp	8.345		Crippen Method
rinpol	2763.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R263024&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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