

3A,17A,20A,21-Tetrahydroxy-5B-pregnan-11-one,

Other names: Cortolone, TMS

tetrakis-TMS
InChI: InChI=1S/C33H66O5Si4/c1-31-19-17-25(36-40(6,7)8)21-24(31)15-16-26-27-18-20-33(38)

InchiKey: LTOJWDHWCDVAFF-XAUXQAQGSA-N

Formula: C33H66O5Si4

SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2C(=O)CC2(C)C1CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)C1

Mol. weight [g/mol]: 655.22

Physical Properties

Property code	Value	Unit	Source
log10ws	0.07		Crippen Method
logp	9.090		Crippen Method
rinpol	3038.00		NIST Webbook
rinpol	3066.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R35901&Units=SI>

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

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/31-712-6/3A-17A-20A-21-Tetrahydroxy-5B-pregnan-11-one-tetrakis-TMS.pdf>

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