

# Pregnan-11-one, 3,17,20,21-tetrakis[(trimethylsilyl)oxy]-, (3«alpha»,5«beta»,20R)-

Other names:

B-Cortolone, 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-FJOVIXCXA-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

CAS: 56196-47-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	0.07		Crippen Method
logp	9.090		Crippen Method
rinpol	3069.00		NIST Webbook
rinpol	3096.00		NIST Webbook

## Sources

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56196475&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

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