

15«beta»,17-Dihydroxypregnanolone, MO-TMS

Inchi: InChI=1S/C31H59NO4Si3/c1-22(32-33-4)31(36-39(11,12)13)21-27(35-38(8,9)10)28-25-1
InchiKey: HGNJIMJEZYWJLX-FICKQYDPSA-N
Formula: C31H59NO4Si3
SMILES: CON=C(C)C1(O[Si](C)(C)C)CC(O[Si](C)(C)C)C2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3
Mol. weight [g/mol]: 594.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	8.612		Crippen Method
rinpol	2746.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R537043&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/40-020-4/15-beta-17-Dihydroxypregnanolone-MO-TMS.pdf>

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