

5«beta»-Pregnane-3«alpha»,17«alpha»,20«alpha» (3-O)-TMTBSi, (17,20-O)-diTMSi

InChI: CC1=1S(C33H66O3Si3)C1=24(34-37(17,18)C33(36-38(10,11)12)22-19-29-27-16-15-25-23
InChIKey: MSYPOULLCDECEM-XQZPXUECSA-N
Formula: C33H66O3Si3
SMILES: CC(O[Si](C)(C)C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C(C)(C)C)CCC4(C)C3C
Mol. weight [g/mol]: 595.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	10.250		Crippen Method
rinpol	3394.00		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=R144295&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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