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

Inchi: InChI=1S/C33H66O3Si3/c1-24(31-27(7,8)9)33(36-38(10,11)12)22-19-29-27-16-15-25-23
InchiKey: MSYPOULLCDECEM-XQEPXUECSA-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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R144295&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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