Pregnenetriol, TMS

Inchi: InChI=1S/C30H58O3Si3/c1-21(31-34(4,5)6)25-15-16-26-24-14-13-22-19-23(32-35(7,8)9)
InchiKey: IHOLKZCGMIBXNK-QTMWDAGXSA-N
Formula: C30H58O3Si3
SMILES: CC(O[Si](C)(C)C)C1CCC2C3CCC4=CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12
Mol. weight [g/mol]: 551.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	8.856		Crippen Method
rinpol	2943.00		NIST Webbook
rinpol	2943.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R36010&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices