5-Pregnen-3«beta»,20«alpha»-diol, TBDMS

Inchi: InChI=1S/C33H62O2Si2/c1-23(34-36(10,11)30(2,3)4)27-16-17-28-26-15-14-24-22-25(35
InchiKey: BUSSZAFGSKFLCU-PLWCNECCSA-N
Formula: C33H62O2Si2
SMILES: CC(O[Si](C)(C)C(C)(C)C)C1CCC2C3CC=C4CC(O[Si](C)(C)C(C)(C)C)CCC4(C)C3CCC1
Mol. weight [g/mol]: 547.02

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.12		Crippen Method
logp	10.366		Crippen Method
rinpol	3417.00		NIST Webbook
rinpol	3417.00		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=R526266&Units=SI

Legend

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