5«beta»-Pregnane-3«alpha»,17«alpha»,20«alpha»-triol-(3,20-O)-diTBDMSi

Inchi: InChI=1S/C33H64O3Si2/c1-23(35-37(10,11)29(2,3)4)33(34)21-18-28-26-15-14-24-22-25

InchiKey: GHNXJGWJFKLUHM-ZNWXLFBDSA-N

Formula: C33H64O3Si2

SMILES: CC(O[Si](C)(C)C(C)(C)C)C1(O)CCC2C3CCC4CC(O[Si](C)(C)C(C)(C)C)CCC4(C)C3CC

Mol. weight [g/mol]: 565.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.64		Crippen Method
logp	9.561		Crippen Method
rinpol	3460.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R144240&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices