5«beta»-Pregnane-3«alpha»,20«alpha»-diol, (3-O)-TMSi, (20-O)-TBDMSi

Inchi: InChI=1S/C30H58O2Si2/c1-21(31-34(10,11)28(2,3)4)25-14-15-26-24-13-12-22-20-23(32

InchiKey: UQRNTCYQNPIFPZ-KGYAFOCASA-N

Formula: C30H58O2Si2

SMILES: CC(O[Si](C)(C)C(C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 506.95

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	9.276		Crippen Method
rinpol	3053.00		NIST Webbook
rinpol	3089.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R144339&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

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