5«beta»-Pregnane-3«alpha»,17«alpha»,20«alpha»(3,17-O)-diTMTBSi,(20-O)-TMSi

Inchi: InChI=1S/C40H76O3Si3/c1-30(42-45(10,11)12)40(43-46(36(2,3)4)27-15-16-28-46)26-21

Inchikey: VZQVHBDHUGHRQR-YMIBEPHVSA-N

Formula: C40H76O3Si3

SMILES: CC(O[Si](C)(C)C)C1(O[Si]2(C(C)(C)C)CCCC2)CCC2C3CCC4CC(OC5([Si](C)(C)C)CCC

Mol. weight [g/mol]: 689.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.85		Crippen Method
logp	12.139		Crippen Method
rinpol	3896.00		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=R385981&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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