5.alpha.-Pregnane-11,20-dione-3.alpha.,21-diol, TMSO-TMS, # 2

Inchi: InChI=1S/C32H64N2O4Si4/c1-32-21-29(33-37-41(8,9)10)31-25-17-15-24(36-40(5,6)7)20

InchiKey: SGEJXYYPQSHIRL-ULPLONOHSA-N

Formula: C32H64N2O4Si4

SMILES: C[C@]12CC(=NO[Si](C)(C)C)C3C(CC[C@H]4C[C@H](O[Si](C)(C)C)CCC34)C1CC[C@

Mol. weight [g/mol]: 653.22

Physical Properties

Property code	Value	Unit	Source
logp	9.352		Crippen Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R526904&Units=SI

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient