3A,17A,21-Trihydroxy-5B-pregnan-11,20-dione, MO TMS

Other names: 5«beta»-Pregnane-3«alpha», 17«alpha», 21-triol-11, 20-dione (THE), MO TMS

Inchi: InChI=1S/C32H62N2O5Si3/c1-30-18-16-24(38-41(8,9)10)20-23(30)14-15-25-26-17-19-3

InchiKey: GRUGCVVBQPMXKS-BCVDSYQDSA-N

Formula: C32H62N2O5Si3

SMILES: CON=C1CC2(C)C(CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)=NOC)C2CCC3CC(O[Si](C)(C)C)

Mol. weight [g/mol]: 639.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	8.306		Crippen Method
rinpol	2978.00		NIST Webbook
rinpol	2982.00		NIST Webbook
rinpol	2960.00		NIST Webbook
rinpol	2977.00		NIST Webbook
rinpol	2977.00		NIST Webbook
rinpol	2965.00		NIST Webbook
rinpol	2983.00		NIST Webbook
rinpol	2960.00		NIST Webbook
rinpol	2983.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R97513&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices