

3,20-Dioxo-11«beta»,18-epoxy-17«alpha»,18,21-trihydroxy-4-pregnene-MO-TMS, syn

InChI: InChI=1S/C32H58N2O6Si3/c1-30-20-26-28-24(14-13-22-19-23(33-35-2)15-17-31(22,28)29-32)/n1-2/p1
InChIKey: PDTVONBIEZWAOH-HSBHMTCHSA-N
Formula: C32H58N2O6Si3
SMILES: CON=C1C=C2CCC3C4C(CC5(C)C3CCC5(O[Si](C)(C)C)C(CO[Si](C)(C)C)=NOC)OC(O[Si](C)(C)C)C2C1
Mol. weight [g/mol]: 651.07

Physical Properties

Property code	Value	Unit	Source
logp	7.562		Crippen Method
rinpol	3228.00		NIST Webbook
rinpol	3228.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R531892&Units=SI>

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

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

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/121-562-3/3-20-Dioxo-11-beta-18-epoxy-17-alpha-18-21-trihydroxy-4-pregnene-MO-TM>

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