Pregn-4-ene-3,20-dione, 11-hydroxy-17,21-bis[(trimethylsilyl)oxy]-, bis(O-methyloxime), (11«beta»)-

Other names: 4-Pregnen-11«beta»,17«alpha»,21-triol-3,20-dione, MO-TMS (11-OH)
Inchi: InChI=1S/C29H52N2O5Si2/c1-27-15-13-21(30-33-3)17-20(27)11-12-22-23-14-16-29(36-
InchiKey: RTBBMHHUSLGXCC-LJAWVBNOSA-N
Formula: C29H52N2O5Si2
SMILES: CON=C1C=C2CCC3C(C(O)CC4(C)C3CCC4(O[Si](C)(C)C)C(CO[Si](C)(C)C)=NOC)C2(C
Mol. weight [g/mol]: 564.90
CAS: 57305-44-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Cheméo Relay (1.0)
logp	6.367		Crippen Method
rinpol	3374.00		NIST Webbook
rinpol	3374.00		NIST Webbook
tf	413.41	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57305449&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):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point