5-Pregnen-3-«beta»-ol-11,20-dione, MO-TMS

Inchi: InChI=1S/C26H44N2O3Si/c1-17(27-29-4)21-11-12-22-20-10-9-18-15-19(31-32(6,7)8)13-
InchiKey: GGPCBFZXZAMTAP-KDNZTQFNSA-N
Formula: C26H44N2O3Si
SMILES: CON=C1CC2(C)C(C(C)=NOC)CCC2C2CC=C3CC(O[Si](C)(C)C)CCC3(C)C12
Mol. weight [g/mol]: 460.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Crippen Method
logp	6.420		Crippen Method
rinpol	2862.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R487215&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