4-Pregnen-20-«alpha»-ol-3,11-dione, MO-TMS

Inchi: InChI=1S/C26H44N2O3Si/c1-17(31-32(6,7)8)21-11-12-22-20-10-9-18-15-19(27-29-4)13-
InchiKey: BCFDIEQJJBSNET-NCUDPPAXSA-N
Formula: C26H44N2O3Si
SMILES: CON=C1C=C2CCC3C(C(=NOC)CC4(C)C(C(C)O[Si](C)(C)C)CCC34)C2(C)CC1
Mol. weight [g/mol]: 460.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Crippen Method
logp	6.420		Crippen Method
rinpol	3022.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R486163&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices