17«alpha»,21-Dihydroxypregn-4-en-3,20-dione, bis-MO-21-TMS(d9)

Inchi: InChI=1S/C26H44N2O4Si/c1-24-13-10-19(27-30-3)16-18(24)8-9-20-21(24)11-14-25(2)22

InchiKey: ZWQYGFFYGLCOFP-CNRRNCJVSA-N

Formula: C26H35D9N2O4Si

SMILES: CON=C1C=C2CCC3C(CCC4(C)C3CCC4(O)C(CO[Si](C)(C)C)=NOC)C2(C)CC1

Mol. weight [g/mol]: 485.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	5.537		Crippen Method
rinpol	3155.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R525065&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