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

Inchi: InChI=1S/C26H46N2O3Si/c1-17(27-29-4)21-11-12-22-20-10-9-18-15-19(31-32(6,7)8)13-

InchiKey: QNTUYUZHRGUGNY-LSXSRRAZSA-N

Formula: C26H46N2O3Si

SMILES: CON=C(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(=NOC)CC12C

Mol. weight [g/mol]: 462.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	6.500		Crippen Method
rinpol	2776.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R487002&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices