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

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

InchiKey: NAHQLWIRZFYOOZ-LZACHHETSA-N

Formula: C26H46N2O3Si

SMILES: CON=C1CCC2(C)C(CCC3C4CCC(C(C)O[Si](C)(C)C)C4(C)CC(=NOC)C32)C1

Mol. weight [g/mol]: 462.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	6.500		Crippen Method
rinpol	2967.00		NIST Webbook
rinpol	2967.00		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=R486445&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices