4-Pregnen-11-«beta»,20-«beta»-diol-3-one, MO-TMS

Inchi: InChI=1S/C28H51NO3Si2/c1-19(31-33(5,6)7)23-13-14-24-22-12-11-20-17-21(29-30-4)15

InchiKey: POLSCKPVKDCQEJ-DGEIVTRFSA-N

Formula: C28H51NO3Si2

SMILES: CON=C1C=C2CCC3C(C(O[Si](C)(C)C)CC4(C)C(C(C)O[Si](C)(C)C)CCC34)C2(C)CC1

Mol. weight [g/mol]: 505.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	7.638		Crippen Method
rinpol	3084.00		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=R486143&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices