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

Inchi: InChI=1S/C28H51NO3Si2/c1-19(31-33(5,6)7)23-13-14-24-22-12-11-20-17-21(32-34(8,9)
InchiKey: DNHGSMBOGFVZQW-IYFUHNTMSA-N
Formula: C28H51NO3Si2
SMILES: CON=C1CC2(C)C(C(C)O[Si](C)(C)C)CCC2C2CCC3=CC(O[Si](C)(C)C)CCC3(C)C12
Mol. weight [g/mol]: 505.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	7.638		Crippen Method
rinpol	2988.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R486272&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