5-«beta»-Pregnan-3-«alpha»,11-«beta»-diol-20-on
MO-TMS

Inchi: InChI=1S/C28H53NO3Si2/c1-19(29-30-4)23-13-14-24-22-12-11-20-17-21(31-33(5,6)7)15
InchiKey: ZGXYWFUBLPJGKA-UTBBBQGXSA-N
Formula: C28H53NO3Si2
SMILES: CON=C(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)CC12C
Mol. weight [g/mol]: 507.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	7.718		Crippen Method
rinpol	2859.00		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=R486965&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices