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

Inchi: InChI=1S/C28H53NO3Si2/c1-19(31-33(5,6)7)23-13-14-24-22-12-11-20-17-21(29-30-4)15
InchiKey: PNHAIJSHVMDURX-AOMDDRBMSA-N
Formula: C28H53NO3Si2
SMILES: CON=C1CCC2(C)C(CCC3C4CCC(C(C)O[Si](C)(C)C)C4(C)CC(O[Si](C)(C)C)C32)C1
Mol. weight [g/mol]: 507.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	7.718		Crippen Method
rinpol	3010.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R486376&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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