5«beta»-Pregnane-3«beta»,17«alpha»-diol-20-one MO TMS

Inchi: InChI=1S/C28H53NO3Si2/c1-20(29-30-4)28(32-34(8,9)10)18-15-25-23-12-11-21-19-22(3

InchiKey: WPPGDMRLWMCELS-GOUXDGQCSA-N

Formula: C28H53NO3Si2

SMILES: CON=C(C)C1(O[Si](C)(C)C)CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C

Mol. weight [g/mol]: 507.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	7.862		Crippen Method
rinpol	2756.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R250538&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