5«alpha»-Pregnane-3«beta», 16«alpha»-diol-20-one, MO TMS

Other names: 16«alpha»-Hydroxypregnanolone, MO TMS
Inchi: InChI=1S/C28H53NO3Si2/c1-19(29-30-4)26-25(32-34(8,9)10)18-24-22-12-11-20-17-21(3
InchiKey: RQHCBMPEWAEMBW-SXWNTBQOSA-N
Formula: C28H53NO3Si2
SMILES: CON=C(C)C1C(O[Si](C)(C)C)CC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 507.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	7.718		Crippen Method
rinpol	2961.00		NIST Webbook
rinpol	2972.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R250370&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