5«alpha»-Pregnan-3«beta»,20«alpha»-diol, VDMS

Inchi: InChI=1S/C28H50O2Si2/c1-9-31(5,6)29-20(3)26-15-16-27-25-13-11-21-19-22(30-32(7,8)

InchiKey: SMVDIMGNHKWSTB-HDTASXAASA-N

Formula: C28H50O2Si2

SMILES: C=C[Si](C)(C)OC1CCC2C(CCC3C2CCC2(C)C(C(C)O[Si](C)(C)C=C)CCC32)C1

Mol. weight [g/mol]: 474.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	7.906		Crippen Method
rinpol	3056.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R529423&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