5-«alpha»-Pregnane-17-«alpha»,20-«beta»,21-triol tris-TMS

Inchi: InChI=1S/C30H60O3Si3/c1-28-19-13-12-14-23(28)15-16-24-25(28)17-20-29(2)26(24)18-

InchiKey: XCHVDXCTEBATMT-KCVPSGEOSA-N

Formula: C30H60O3Si3

SMILES: CC12CCCCC1CCC1C2CCC2(C)C1CCC2(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C

Mol. weight [g/mol]: 553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Crippen Method
logp	9.081		Crippen Method
rinpol	2870.00		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=R149809&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices