5-«alpha»-Pregnane-3-«beta»,17-«alpha»,20-«beta»-triol-tris-TMS

Inchi: InChI=1S/C30H60O3Si3/c1-22(31-34(4,5)6)30(33-36(10,11)12)20-17-27-25-14-13-23-21

InchiKey: KFUWLVZCEDFJIK-YHQIZCJDSA-N

Formula: C30H60O3Si3

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

Mol. weight [g/mol]: 553.05

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.26		Crippen Method
logp	9.079		Crippen Method
rinpol	2950.00		NIST Webbook
rinpol	2950.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R150022&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