5«alpha»-Androstan-6«beta»-ol-3,17-dione,tris-TM

Inchi: InChI=1S/C28H52O3Si3/c1-27-16-14-20(29-32(3,4)5)18-24(27)25(30-33(6,7)8)19-21-22-
InchiKey: ZNMLKZDNEJOGCO-BPSSBHKSSA-N
Formula: C28H52O3Si3
SMILES: CC12CCC3C(CC(O[Si](C)(C)C)C4CC(O[Si](C)(C)C)=CCC43C)C1CC=C2O[Si](C)(C)C
Mol. weight [g/mol]: 520.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.90		Crippen Method
logp	8.550		Crippen Method
rinpol	2745.00		NIST Webbook
rinpol	2750.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R319261&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