Androsta-1,4-dien-6«beta»-ol-3,17-dione,tris-TMS

Inchi: InChI=1S/C28H48O3Si3/c1-27-16-14-20(29-32(3,4)5)18-24(27)25(30-33(6,7)8)19-21-22-
InchiKey: JNXWIUXKBXITAT-FJXIBAFOSA-N
Formula: C28H48O3Si3
SMILES: CC12C=CC(O[Si](C)(C)C)=CC1=C(O[Si](C)(C)C)CC1C2CCC2(C)C(O[Si](C)(C)C)=CCC
Mol. weight [g/mol]: 516.94

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	8.595		Crippen Method
rinpol	2820.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R319434&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