«beta»-Cortolone, tris-TMS

Inchi: InChI=1S/C30H58O5Si3/c1-28-16-14-22(34-37(6,7)8)18-21(28)12-13-23-24-15-17-30(32
InchiKey: RPGCPBZHXIDXGQ-HVZZIZDUSA-N
Formula: C30H58O5Si3
SMILES: CC12CCC(O[Si](C)(C)C)CC1CCC1C2C(=O)CC2(C)C1CCC2(O)C(CO[Si](C)(C)C)O[Si](C
Mol. weight [g/mol]: 583.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.80		Crippen Method
logp	7.231		Crippen Method
rinpol	3092.00		NIST Webbook
rinpol	3092.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R16527&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices