Allopregnanediol TMS

Inchi: InChI=1S/C28H54O2Si2/c1-10-26(30-32(7,8)9)25-14-13-23-22-12-11-20-19-21(29-31(4,5
InchiKey: FFOITQMJIMFGSD-BBEQGNITSA-N
Formula: C28H54O2Si2
SMILES: CCC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 478.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	8.495		Crippen Method
rinpol	2783.00		NIST Webbook
rinpol	2796.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R97620&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