24R,25-Dihydroxycholecalciferol, butylboronate, 3-TMS, # 1

Inchi: InChI=1S/C34H59BO3Si/c1-10-11-23-35-36-32(33(4,5)38-35)21-15-26(3)30-19-20-31-27

InchiKey: JQLCKMRAFHGTRV-GPMKEHIUSA-N

Formula: C34H59BO3Si

SMILES: C=C1CCC(O[Si](C)(C)C)CC1=CC=C1CCCC2(C)C1CCC2C(C)CCC1OB(CCCC)OC1(C)C

Mol. weight [g/mol]: 554.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.54		Crippen Method
logp	9.914		Crippen Method
rinpol	3453.00		NIST Webbook
rinpol	3453.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R529230&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