24R,25-Dihydroxycholecalciferol, methylboronate, 3-TBDMS, # 2

Inchi: InChI=1S/C34H59BO3Si/c1-24-14-18-28(37-39(10,11)32(3,4)5)23-27(24)17-16-26-13-12

InchiKey: WHTZOZCCVNIKJO-RKTWTOSESA-N

Formula: C34H59BO3Si

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

Mol. weight [g/mol]: 554.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.54		Crippen Method
logp	9.914		Crippen Method
rinpol	3550.00		NIST Webbook
rinpol	3550.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R529265&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices