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

Inchi: InChI=1S/C31H53BO3Si/c1-22-12-16-26(34-36(7,8)9)21-25(22)15-14-24-11-10-20-31(5)
InchiKey: VDXTWINWWUCBMW-PKVCTLIISA-N
Formula: C31H53BO3Si
SMILES: C=C1CCC(O[Si](C)(C)C)CC1=CC=C1CCCC2(C)C1CCC2C(C)CCC1OB(C)OC1(C)C
Mol. weight [g/mol]: 512.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.29		Crippen Method
logp	8.744		Crippen Method
rinpol	3122.00		NIST Webbook
rinpol	3122.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R529270&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