

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

**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	3276.00		NIST Webbook
rinpol	3276.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529285&Units=SI>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/23-341-7/24R-25-Dihydroxycholecalciferol-methylboronate-3-TMS-2.pdf>

Generated by Cheméo on 2024-04-25 19:03:21.993610896 +0000 UTC m=+16361050.914188266.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.