

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)
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

Latest version available from:

<https://www.chemeo.com/cid/70-039-1/24R-25-Dihydroxycholecalciferol-butylboronate-3-TMS-1.pdf>

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