

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

Inchi: InChI=1S/C37H65BO3Si/c1-12-13-25-38-39-34(36(7,8)41-38)23-17-28(3)32-21-22-33-29
InchiKey: YYAMBCYDCSYASL-KVXRBUDUSA-N
Formula: C37H65BO3Si
SMILES: C=C1CCC(O[Si](C)(C)C(C)(C)C)CC1=CC=C1CCCC2(C)C1CCC2C(C)CCC1OB(CCCC)
Mol. weight [g/mol]: 596.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.80		Crippen Method
logp	11.085		Crippen Method
rinpol	3845.00		NIST Webbook
rinpol	3845.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529225&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/124-578-3/24R-25-Dihydroxycholecalciferol-butylboronate-3-TBDMS-2.pdf>

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