

24R,25-Dihydroxycholecalciferol, tris-TMS, # 1

Inchi: InChI=1S/C36H68O3Si3/c1-27-17-21-31(37-40(6,7)8)26-30(27)20-19-29-16-15-25-36(5)
InchiKey: QYCXEPMWUJWGBH-JKKBKWPTRSA-N
Formula: C36H68O3Si3
SMILES: C=C1CCC(O[Si](C)(C)C)CC1=CC=C1CCCC2(C)C1CCC2C(C)CCC(O[Si](C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 633.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	11.282		Crippen Method
rinpol	3434.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529290&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

Latest version available from:

<https://www.chemeo.com/cid/50-783-7/24R-25-Dihydroxycholecalciferol-tris-TMS-1.pdf>

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