7-angelyl echinatine, diTMS, dihydro

Inchi: InChI=1S/C26H49NO6Si2/c1-12-19(4)24(28)31-22-14-16-27-15-13-21(23(22)27)17-30-2
InchiKey: PKEAGNHRNFCIQF-SRXDOAFQSA-N
Formula: C26H49NO6Si2
SMILES: CC=C(C)C(=O)OC1CCN2CCC(COC(=O)C(O[Si](C)(C)C)(C(C)C)C(C)C)C(C)O[Si](C)(C)C12
Mol. weight [g/mol]: 527.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.88		Crippen Method
logp	4.988		Crippen Method
rinpol	2673.00		NIST Webbook
rinpol	2673.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R252381&Units=SI

Legend

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