«beta»-angelyl echinatine, diTMS

Inchi: InChI=1S/C26H47NO6Si2/c1-12-19(4)24(28)31-20(5)26(18(2)3,33-35(9,10)11)25(29)30-
InchiKey: TXFNCHBEQLHJRR-YENBOYLJSA-N
Formula: C26H47NO6Si2
SMILES: CC=C(C)C(=O)OC(C)C(O[Si](C)(C)C)(C(=O)OCC1=CCN2CCC(O[Si](C)(C)C)C12)C(C)C
Mol. weight [g/mol]: 525.83

Physical Properties

Property code	Value	Unit	Source
logp	4.908		Crippen Method
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R252316&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices