7-acetyl echinatine, diTMS

Inchi: InChI=1S/C23H43NO6Si2/c1-16(2)23(30-32(8,9)10,17(3)29-31(5,6)7)22(26)27-15-19-11
InchiKey: UHYXQSGPEXMCCX-PIBIMKELSA-N
Formula: C23H43NO6Si2
SMILES: CC(=O)OC1CCN2CC=C(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]: 485.76

Physical Properties

Property code	Value	Unit	Source
log10ws	0.13		Crippen Method
logp	3.962		Crippen Method
rinpol	2428.00		NIST Webbook
rinpol	2428.00		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=R252361&Units=SI

Legend

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