3-Methyl-2-butenyl-3-acetyloxycaffeate, TMS

Inchi: InChI=1S/C22H34O6Si2/c1-16(2)12-13-25-21(24)11-10-18-14-19(26-17(3)23)22(28-30(7
InchiKey: UZYCIVYKDKQUMK-ZHACJKMWSA-N
Formula: C22H34O6Si2
SMILES: CC(=O)Oc1cc(C=CC(=O)OCC=C(C)C)cc(O[Si](C)(C)C)c1O[Si](C)(C)C
Mol. weight [g/mol]: 450.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	5.562		Crippen Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R403004&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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