3-Methyl-2-butenyl (E)-3-acetylcaffeate, TMS

Inchi: InChI=1S/C19H26O5Si/c1-14(2)11-12-22-19(21)10-8-16-7-9-17(24-25(4,5)6)18(13-16)23
InchiKey: MYDGGGPTAPMVDB-CSKARUKUSA-N
Formula: C19H26O5Si
SMILES: CC(=O)Oc1cc(C=CC(=O)OCC=C(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 362.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	4.348		Crippen Method
rinpol	2458.00		NIST Webbook
rinpol	2458.00		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=R173050&Units=SI

Legend

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