Benzyl (E)-3-acetylcaffeate, TMS

Inchi: InChI=1S/C21H24O5Si/c1-16(22)25-20-14-17(10-12-19(20)26-27(2,3)4)11-13-21(23)24-
InchiKey: RMSLYNNTKQUDOY-ACCUITESSA-N
Formula: C21H24O5Si
SMILES: CC(=O)Oc1cc(C=CC(=O)OCc2ccccc2)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 384.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	4.582		Crippen Method
rinpol	2783.00		NIST Webbook
rinpol	2783.00		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=R173114&Units=SI

Legend

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