2-Phenylethyl (E)-4-acetylcaffeate, TMS

Inchi: InChI=1S/C22H26O5Si/c1-17(23)26-20-12-10-19(16-21(20)27-28(2,3)4)11-13-22(24)25-
InchiKey: HVUYHWOOMSKJCN-ACCUITESSA-N
Formula: C22H26O5Si
SMILES: CC(=O)Oc1ccc(C=CC(=O)OCCc2ccccc2)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 398.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	4.625		Crippen Method
rinpol	2785.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R173030&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