(E)-3-Acetylcaffeic acid, bis-TMS

Inchi: InChI=1S/C17H26O5Si2/c1-13(18)20-16-12-14(8-10-15(16)21-23(2,3)4)9-11-17(19)22-24
InchiKey: DTDLRMHGRMYLHL-PKNBQFBNSA-N
Formula: C17H26O5Si2
SMILES: CC(=O)Oc1cc(C=CC(=O)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 366.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.20		Crippen Method
logp	4.217		Crippen Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		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=R173149&Units=SI

Legend

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