Cinnamyl (E)-p-coumarate, mono-TMS

Inchi: InChI=1S/C21H24O3Si/c1-25(2,3)24-20-14-11-19(12-15-20)13-16-21(22)23-17-7-10-18-
InchiKey: XUHDHAHIDPZOOL-NJKRNUQASA-N
Formula: C21H24O3Si
SMILES: C[Si](C)(C)Oc1ccc(C=CC(=O)OCC=Cc2ccccc2)cc1
Mol. weight [g/mol]: 352.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	5.170		Crippen Method
rinpol	2794.00		NIST Webbook
rinpol	2794.00		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=R315823&Units=SI

Legend

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