Phenylethyl (E)-caffeate, bis-TMS

Other names:	2-Phenylethyl (E)-caffeate, TMS
	2-Phenylethyl caffeate, TMS
Inchi:	InChI=1S/C23H32O4Si2/c1-28(2,3)26-21-14-12-20(18-22(21)27-29(4,5)6)13-15-23(24)25
InchiKey:	YIRGTBZPWJGXDB-FYWRMAATSA-N
Formula:	C23H32O4Si2
SMILES:	C[Si](C)(C)Oc1ccc(C=CC(=O)OCCc2ccccc2)cc1O[Si](C)(C)C
Mol. weight [g/mol]:	428.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	5.913		Crippen Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R55921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient