2-Methylpropyl (E)-isoferulate, TMS

Inchi:	InChI=1S/C17H26O4Si/c1-13(2)12-20-17(18)10-8-14-7-9-15(19-3)16(11-14)21-22(4,5)6/
InchiKey:	QCUKNNMYAGJGQQ-CSKARUKUSA-N
Formula:	C17H26O4Si
SMILES:	COc1ccc(C=CC(=O)OCC(C)C)cc1O[Si](C)(C)C
Mol. weight [g/mol]:	322.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	4.121		Crippen Method
rinpol	2149.00		NIST Webbook
rinpol	2149.00		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=R42198&Units=SI

Legend

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

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