3-Methylbutyl (E)-isoferulate, TMS

Inchi: InChI=1S/C18H28O4Si/c1-14(2)11-12-21-18(19)10-8-15-7-9-16(20-3)17(13-15)22-23(4,5
InchiKey: MOFQCEGVUYCISG-CSKARUKUSA-N
Formula: C18H28O4Si
SMILES: COc1ccc(C=CC(=O)OCCC(C)C)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 336.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	4.511		Crippen Method
rinpol	2255.00		NIST Webbook
rinpol	2255.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R42273&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