2-phenylethylglucosinolate, TMS

Inchi: InChI=1S/C30H61NO9S2Si5/c1-43(2,3)34-23-25-27(36-44(4,5)6)28(37-45(7,8)9)29(38-4
InchiKey: KFICNUSQTQVFON-UHFFFAOYSA-N
Formula: C30H61NO9S2Si5
SMILES: C[Si](C)(C)OCC1OC(SC(CCc2ccccc2)=NOS(=O)(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[
Mol. weight [g/mol]: 784.36

Physical Properties

Property code	Value	Unit	Source
log10ws	2.35		Crippen Method
logp	8.016		Crippen Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R383970&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
rinpol: Non-polar retention indices