2-hydroxy-2-phenylethyl glucosinolate, TMS

Inchi: InChI=1S/C33H69NO10S2Si6/c1-47(2,3)37-25-28-30(40-49(7,8)9)31(41-50(10,11)12)32
InchiKey: FKKXAOUNEDKCJU-UHFFFAOYSA-N
Formula: C33H69NO10S2Si6
SMILES: C[Si](C)(C)OCC1OC(SC(CC(O[Si](C)(C)C)c2ccccc2)=NOS(=O)(=O)O[Si](C)(C)C)C(O[Si
Mol. weight [g/mol]: 872.54

Physical Properties

Property code	Value	Unit	Source
log10ws	3.50		Crippen Method
logp	9.366		Crippen Method
rinpol	2847.00		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=R383965&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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