2-hydroxy-2-methylpropyl glucosinolate, TMS

Inchi: InChI=1S/C29H69NO10S2Si6/c1-29(2,38-47(15,16)17)21-24(30-39-42(31,32)40-48(18,1
InchiKey: WTWNHNZNNVNNQK-UHFFFAOYSA-N
Formula: C29H69NO10S2Si6
SMILES: CC(C)(CC(=NOS(=O)(=O)O[Si](C)(C)C)SC1OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C
Mol. weight [g/mol]: 824.50

Physical Properties

Property code	Value	Unit	Source
log10ws	4.63		Crippen Method
logp	8.403		Crippen Method
rinpol	2551.00		NIST Webbook
rinpol	2551.00		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=R383950&Units=SI

Legend

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