p-hydroxybenzyl glucosinolate, TMS

Inchi: InChI=1S/C32H67NO10S2Si6/c1-46(2,3)36-24-27-29(39-48(7,8)9)30(40-49(10,11)12)31
InchiKey: LJQFSWLBQFBCQA-MDVFONAFSA-N
Formula: C32H67NO10S2Si6
SMILES: C[Si](C)(C)OCC1OC(SC(Cc2ccc(O[Si](C)(C)C)cc2)=NOS(=O)(=O)O[Si](C)(C)C)C(O[Si](
Mol. weight [g/mol]: 858.52

Physical Properties

Property code	Value	Unit	Source
log10ws	3.76		Crippen Method
logp	8.839		Crippen Method
rinpol	2942.00		NIST Webbook
rinpol	2942.00		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=R384022&Units=SI

Legend

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