3-butenyl glucosinolate, TMS

Inchi: InChI=1S/C26H59NO9S2Si5/c1-17-18-19-22(27-35-38(28,29)36-43(14,15)16)37-26-25(3
InchiKey: SOAXBYFVOFWXQV-UHFFFAOYSA-N
Formula: C26H59NO9S2Si5
SMILES: C=CCCC(=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]: 734.30

Physical Properties

Property code	Value	Unit	Source
log10ws	3.28		Crippen Method
logp	7.349		Crippen Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R383985&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

Latest version available from:
https://www.chemeo.com/cid/56-800-1/3-butenyl-glucosinolate-TMS.pdf
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