

2-hydroxy-3-butenyl glucosinolate, TMS

Other names:	Glucosinolate, 2-hydroxy-3-butenyl, TMS
Inchi:	InChI=1S/C29H67NO7SSi6/c1-20-23(33-40(5,6)7)21-25(30-37-44(17,18)19)38-29-28(36
InchiKey:	LDECHQMANAQQFL-UHFFFAOYSA-N
Formula:	C29H67NO7SSi6
SMILES:	C=CC(CC(=NO[Si](C)(C)C)SC1OC(CO[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O
Mol. weight [g/mol]:	742.42

Physical Properties

Property code	Value	Unit	Source
log10ws	4.67		Crippen Method
logp	8.917		Crippen Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R53931&Units=SI

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/50-882-7/2-hydroxy-3-butenyl-glucosinolate-TMS.pdf>

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