Allyl glucosinolate, TMS

Inchi:	InChI=1S/C25H57NO9S2Si5/c1-17-18-21(26-34-37(27,28)35-42(14,15)16)36-25-24(33-4
InchiKey:	NPNBNHMLOAYHIJ-UHFFFAOYSA-N
Formula:	C25H57NO9S2Si5
SMILES:	C=CCC(=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]:	720.28

Physical Properties

Property code	Value	Unit	Source
log10ws	3.70		Crippen Method
logp	6.959		Crippen Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		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=R383990&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/51-962-7/Allyl-glucosinolate-TMS.pdf
Generated by Cheméo on 2024-04-18 17:23:15.767849176 +0000 UTC m=+15750244.688426498.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.