

Glucosinolate, 4-pentenyl, TMS

Other names:	4-pentenyl glucosinolate, TMS
Inchi:	InChI=1S/C27H61NO6SSi5/c1-17-18-19-20-23(28-34-40(14,15)16)35-27-26(33-39(11,12)13)24-25
InchiKey:	SRWUAGXHILMRIM-UHFFFAOYSA-N
Formula:	C27H61NO6SSi5
SMILES:	C=CCCCC(=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]:	668.27

Physical Properties

Property code	Value	Unit	Source
log10ws	2.76		Crippen Method
logp	8.478		Crippen Method
rinsol	2482.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R54018&Units=SI

Legend

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

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<https://www.cheméo.com/cid/25-720-4/Glucosinolate-4-pentenyl-TMS.pdf>

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