

2-phenylethylglucosinolate, TMS

Inchi:	InChI=1S/C30H61NO9S2Si5/c1-43(2,3)34-23-25-27(36-44(4,5)6)28(37-45(7,8)9)29(38-4
InchiKey:	KFICNUSQTQVFON-UHFFFAOYSA-N
Formula:	C ₃₀ H ₆₁ N _O S ₂ Si ₅
SMILES:	C[Si](C)(C)OCC1OC(SC(CCc2ccccc2)=NOS(=O)(=O)O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)
Mol. weight [g/mol]:	784.36

Physical Properties

Property code	Value	Unit	Source
log10ws	2.35		Crippen Method
logp	8.016		Crippen Method
rinpol	2820.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R383970&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/25-996-9/2-phenylethylglucosinolate-TMS.pdf>

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