Glyceollin I, TMS

Inchi:	InChI=1S/C26H34O5Si2/c1-25(2)14-13-18-21(29-25)12-10-19-23(18)27-16-26(31-33(6,7
InchiKey:	FSNDGZURVHLRTH-RSXGOPAZSA-N
Formula:	C26H34O5Si2
SMILES:	CC1(C)C=Cc2c(ccc3c2OCC2(O[Si](C)(C)C)c4ccc(O[Si](C)(C)C)cc4OC32)O1
Mol. weight [g/mol]:	482.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	6.657		Crippen Method

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=R299182&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

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https://www.chemeo.com/cid/91-606-8/Glyceollin-I-TMS.pdf

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