Glyceollin V, TMS

Inchi:	InChI=1S/C26H36O5Si2/c1-16(2)21-12-17-11-19-23(14-22(17)28-21)27-15-26(31-33(6,7
InchiKey:	QWOKOHGVXXLYIF-BYXVTNLJSA-N
Formula:	C26H36O5Si2
SMILES:	CC(C)C1Cc2cc3c(cc2O1)OCC1(O[Si](C)(C)C)c2ccc(O[Si](C)(C)C)cc2OC31
Mol. weight [g/mol]:	484.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.05		Crippen Method
logp	6.433		Crippen Method
rinpol	2896.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R299197&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/70-797-0/Glyceollin-V-TMS.pdf

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