

Glyceollin II, TMS

Inchi: InChI=1S/C26H34O5Si2/c1-25(2)12-11-17-13-19-22(15-21(17)29-25)27-16-26(31-33(6,7
InchiKey: JOCQMDAHZUHEAO-RSXGOPAZSA-N
Formula: C26H34O5Si2
SMILES: CC1(C)C=Cc2cc3c(cc2O1)OCC1(O[Si](C)(C)C)c2ccc(O[Si](C)(C)C)cc2OC31
Mol. weight [g/mol]: 482.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	6.657		Crippen Method
rinpol	2805.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R299177&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/91-449-3/Glyceollin-II-TMS.pdf>

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