geranial oxypeucedaninyl acetal (diastereomer b)

Inchi: InChI=1S/C26H30O6/c1-16(2)7-6-8-17(3)13-24-31-22(26(4,5)32-24)15-29-25-18-9-10-23

InchiKey: BXLDUXXKMXZUSB-GHRIWEEISA-N

Formula: C26H30O6

SMILES: CC(C)=CCCC(C)=CC1OC(COc2c3ccoc3cc3oc(=O)ccc23)C(C)(C)O1

Mol. weight [g/mol]: 438.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-16.56		Crippen Method
logp	6.131		Crippen Method
mcvol	334.580	ml/mol	McGowan Method
rinpol	3448.00		NIST Webbook
rinpol	3448.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R422347&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.