

neral oxypeucedaninyl acetal (diastereomer a)

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-LGMDPLHJSA-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	3377.00		NIST Webbook
rinpol	3377.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422392&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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