(R)-9-(2,3-Dihydroxy-3-methylbutoxy)-4-methoxy-

Other names:	7H-Furo(3,2-g)(1)benzopyran-7-one, 9-(2,3-dihydroxy-3-methylbutoxy)-4-methoxy-, (R)-
	Biacangelicin
	Bjacangelicin
	Bjakangelicin
	Byakangelicin
	(+)-Byakangelicin
	Byankagelicine
Inchi:	InChI=1S/C17H18O7/c1-17(2,20)11(18)8-23-16-14-10(6-7-22-14)13(21-3)9-4-5-12(19)24
InchiKey:	PKRPFNXROFUNDE-LLVKDONJSA-N
Formula:	C17H18O7
SMILES:	COc1c2ccoc2c(OCC(O)C(C)(C)O)c2oc(=O)ccc12
Mol. weight [g/mol]:	334.32
CAS:	482-25-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.64		Crippen Method
logp	2.058		Crippen Method
mcvol	233.100	ml/mol	McGowan Method
rinpol	2915.80		NIST Webbook
rinpol	2915.80		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C482257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices