

5-(3',4'-Carbonyldioxyphenyl)-3-isopropyl-2-oxazolidinone

Inchi:	InChI=1S/C13H13NO5/c1-7(2)14-6-11(17-12(14)15)8-3-4-9-10(5-8)19-13(16)18-9/h3-5,7
InchiKey:	TYZQRRNMKWCMMA-UHFFFAOYSA-N
Formula:	C13H13NO5
SMILES:	CC(C)N1CC(c2ccc3oc(=O)oc3c2)OC1=O
Mol. weight [g/mol]:	263.25
CAS:	23271-77-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.52		Crippen Method
logp	2.288		Crippen Method
mcvol	179.280	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23271774&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
mcvol:	McGowan's characteristic volume

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