

2-[5-methoxy-2-methyl-1-(3-phenylprop-2-enoyl)in

Inchi:
acid

InChI=1S/C21H19NO4/c1-14-17(13-21(24)25)18-12-16(26-2)9-10-19(18)22(14)20(23)11

InchiKey:

NKPPORKKCMYYTO-UHFFFAOYSA-N

Formula:

C21H19NO4

SMILES:

COc1ccc2c(c1)c(CC(=O)O)c(C)n2C(=O)C=Cc1ccccc1

Mol. weight [g/mol]:

349.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.54		Aqueous Solubility Prediction Method
logp	3.939		Crippen Method
mcvol	264.630	ml/mol	McGowan Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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