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

Inchi: 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/ci990307l
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