methyl 1-[2-(benzoyloxy)acetyl]pyrrolidine-2-carboxylate

Inchi: InChI=1S/C15H17NO5/c1-20-15(19)12-8-5-9-16(12)13(17)10-21-14(18)11-6-3-2-4-7-11/h

InchiKey: UQIKOYWGLUXMNE-UHFFFAOYSA-N

Formula: C15H17NO5

SMILES: COC(=O)C1CCCN1C(=O)COC(=O)c1ccccc1

Mol. weight [g/mol]: 291.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.08		Aqueous Solubility Prediction Method
logp	1.007		Crippen Method
mcvol	214.020	ml/mol	McGowan Method
tf	345.65	K	Aqueous Solubility Prediction Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

tf: Normal melting (fusion) point

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.