[2-(2-carbamoylpyrrolidin-1-yl)-2-oxoethyl] benzoate

Inchi: InChI=1S/C14H16N2O4/c15-13(18)11-7-4-8-16(11)12(17)9-20-14(19)10-5-2-1-3-6-10/h1

InchiKey: QUIKDFWIKDMXIO-UHFFFAOYSA-N

Formula: C14H16N2O4

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

Mol. weight [g/mol]: 276.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.04		Aqueous Solubility Prediction Method
logp	0.320		Crippen Method
mcvol	204.040	ml/mol	McGowan Method
tf	467.65	K	Aqueous Solubility Prediction Method

Sources

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point

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