(2-oxo-2-pyrrolidin-1-ylethyl) benzoate

Inchi: InChI=1S/C13H15NO3/c15-12(14-8-4-5-9-14)10-17-13(16)11-6-2-1-3-7-11/h1-3,6-7H,4-5

InchiKey: GILNGPKTMRSQDW-UHFFFAOYSA-N

Formula: C13H15NO3

SMILES: O=C(OCC(=O)N1CCCC1)c1ccccc1

Mol. weight [g/mol]: 233.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.57		Aqueous Solubility Prediction Method
logp	1.466		Crippen Method
mcvol	178.400	ml/mol	McGowan 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