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

Inchi: InChI=1S/C14H17NO3/c16-13(15-9-5-2-6-10-15)11-18-14(17)12-7-3-1-4-8-12/h1,3-4,7-8
InchiKey: BCNWJNNKUUMDHS-UHFFFAOYSA-N
Formula: C14H17NO3
SMILES: O=C(OCC(=O)N1CCCCC1)c1ccccc1
Mol. weight [g/mol]: 247.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Aqueous Solubility Prediction Method
logp	1.856		Crippen Method
mcvol	192.490	ml/mol	McGowan 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