

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

<b>Inchi:</b>	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
<b>InchiKey:</b>	BCNWJNNKUUMDHS-UHFFFAOYSA-N
<b>Formula:</b>	C14H17NO3
<b>SMILES:</b>	O=C(OCC(=O)N1CCCCC1)c1ccccc1
<b>Mol. weight [g/mol]:</b>	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/AqueousDataset002.xlsx>

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

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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