

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

<b>Inchi:</b>	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
<b>InchiKey:</b>	GILNGPKTMRSQDW-UHFFFAOYSA-N
<b>Formula:</b>	C13H15NO3
<b>SMILES:</b>	O=C(OCC(=O)N1CCCC1)c1ccccc1
<b>Mol. weight [g/mol]:</b>	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

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## 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

Latest version available from:

<https://www.cheméo.com/cid/106-999-6/2-oxo-2-pyrrolidin-1-ylethyl-benzoate.pdf>

Generated by Cheméo on 2024-05-02 09:16:58.669498351 +0000 UTC m=+16930667.590075661.

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