[2-(4-hydroxypiperidin-1-yl)-2-oxoethyl] benzoate

Inchi: InChI=1S/C14H17NO4/c16-12-6-8-15(9-7-12)13(17)10-19-14(18)11-4-2-1-3-5-11/h1-5,12

InchiKey: YVWZWRFAFZRJGU-UHFFFAOYSA-N

Formula: C14H17NO4

SMILES: O=C(OCC(=O)N1CCC(O)CC1)c1ccccc1

Mol. weight [g/mol]: 263.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Aqueous Solubility Prediction Method
logp	0.827		Crippen Method
mcvol	198.360	ml/mol	McGowan Method
tf	394.65	K	Aqueous Solubility Prediction 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

tf: Normal melting (fusion) point

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