[2-(azepan-1-yl)-2-oxoethyl] benzoate

Inchi: InChI=1S/C15H19NO3/c17-14(16-10-6-1-2-7-11-16)12-19-15(18)13-8-4-3-5-9-13/h3-5,8-

InchiKey: FZBXGZBXWFNCQY-UHFFFAOYSA-N

Formula: C15H19NO3

SMILES: O=C(OCC(=O)N1CCCCCC1)c1ccccc1

Mol. weight [g/mol]: 261.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Aqueous Solubility Prediction Method
logp	2.246		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
tf	380.65	K	Aqueous Solubility Prediction 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

tf: Normal melting (fusion) point

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