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

Inchi: InChI=1S/C12H13NO3/c14-11(13-7-4-8-13)9-16-12(15)10-5-2-1-3-6-10/h1-3,5-6H,4,7-9H
InchiKey: RSDMFNVRFBIYRK-UHFFFAOYSA-N
Formula: C12H13NO3
SMILES: O=C(OCC(=O)N1CCC1)c1ccccc1
Mol. weight [g/mol]: 219.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Aqueous Solubility Prediction Method
logp	1.076		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
tf	347.65	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

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