(2-morpholin-4-yl-2-oxoethyl) benzoate

Inchi: InChI=1S/C13H15NO4/c15-12(14-6-8-17-9-7-14)10-18-13(16)11-4-2-1-3-5-11/h1-5H,6-1
InchiKey: AVZVLGDSSQKRGL-UHFFFAOYSA-N
Formula: C13H15NO4
SMILES: O=C(OCC(=O)N1CCOCC1)c1ccccc1
Mol. weight [g/mol]: 249.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Aqueous Solubility Prediction Method
logp	0.702		Crippen Method
mcvol	184.270	ml/mol	McGowan Method
tf	376.65	K	Aqueous Solubility Prediction Method

Sources

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

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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