[2-(2,6-dimethylpiperidin-1-yl)-2-oxoethyl] benzoate

Inchi: InChI=1S/C16H21NO3/c1-12-7-6-8-13(2)17(12)15(18)11-20-16(19)14-9-4-3-5-10-14/h3-5

InchiKey: WJUSVIUZCYELMK-UHFFFAOYSA-N

Formula: C16H21NO3

SMILES: CC1CCCC(C)N1C(=O)COC(=O)c1ccccc1

Mol. weight [g/mol]: 275.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Aqueous Solubility Prediction Method
logp	2.633		Crippen Method
mcvol	220.670	ml/mol	McGowan 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