

[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/ci9903071>
Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
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

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