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

Inchi: InChI=1S/C16H21NO3/c1-2-14-10-6-7-11-17(14)15(18)12-20-16(19)13-8-4-3-5-9-13/h3-5
InchiKey: WXHDYGRKHGIEOF-UHFFFAOYSA-N
Formula: C16H21NO3
SMILES: CCC1CCCCN1C(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 275.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Aqueous Solubility Prediction Method
logp	2.635		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
tf	327.65	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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