3-Pentanoyloxymethylphenytoin

Other names: [2,5-dioxo-4,4-di(phenyl)imidazolidin-1-yl]methyl pentanoate
Inchi: InChI=1S/C21H22N2O4/c1-2-3-14-18(24)27-15-23-19(25)21(22-20(23)26,16-10-6-4-7-11
InchiKey: XCEYNQCFXXAOBL-UHFFFAOYSA-N
Formula: C21H22N2O4
SMILES: CCCCC(=O)OCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]: 366.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.95		Aqueous Solubility Prediction Method
log10ws	-4.68		Estimated Solubility Method
logp	3.173		Crippen Method
mcvol	278.910	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume