3-Octanoyloxymethylphenytoin

Inchi: InChI=1S/C24H28N2O4/c1-2-3-4-5-12-17-21(27)30-18-26-22(28)24(25-23(26)29,19-13-8
InchiKey: IDZYLIZKJFAXAS-UHFFFAOYSA-N
Formula: C24H28N2O4
SMILES: CCCCCCCC(=O)OCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]: 408.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.52		Aqueous Solubility Prediction Method
log10ws	-6.52		Estimated Solubility Method
logp	4.343		Crippen Method
mcvol	321.180	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

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