3-Heptanoyloxymethylphenytoin

Inchi: InChI=1S/C23H26N2O4/c1-2-3-4-11-16-20(26)29-17-25-21(27)23(24-22(25)28,18-12-7-5
InchiKey: FFGKFDRZZAJYCH-UHFFFAOYSA-N
Formula: C23H26N2O4
SMILES: CCCCCCC(=O)OCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]: 394.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.30		Estimated Solubility Method
logp	3.953		Crippen Method
mcvol	307.090	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

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