3-Propanoyloxymethylphenytoin

Other names: [2,5-dioxo-4,4-di(phenyl)imidazolidin-1-yl]methyl propanoate
Inchi: InChI=1S/C19H18N2O4/c1-2-16(22)25-13-21-17(23)19(20-18(21)24,14-9-5-3-6-10-14)15
InchiKey: FBQTWGHLMQUOQL-UHFFFAOYSA-N
Formula: C19H18N2O4
SMILES: CCC(=O)OCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]: 338.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.98		Aqueous Solubility Prediction Method
log10ws	-4.91		Estimated Solubility Method
logp	2.393		Crippen Method
mcvol	250.730	ml/mol	McGowan Method
tf	443.75	K	Aqueous Solubility Prediction Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point