3-Ethanoyloxymethylphenytoin

Other names: [2,5-dioxo-4,4-di(phenyl)imidazolidin-1-yl]methyl acetate
Inchi: InChI=1S/C18H16N2O4/c1-13(21)24-12-20-16(22)18(19-17(20)23,14-8-4-2-5-9-14)15-10
InchiKey: FBFCVJNZKBVVRP-UHFFFAOYSA-N
Formula: C18H16N2O4
SMILES: CC(=O)OCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]: 324.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Aqueous Solubility Prediction Method
log10ws	-4.47		Estimated Solubility Method
logp	2.003		Crippen Method
mcvol	236.640	ml/mol	McGowan Method
tf	431.25	K	Aqueous Solubility Prediction 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
tf: Normal melting (fusion) point