3-Butanoyloxymethylphenytoin

Other names: [2,5-dioxo-4,4-di(phenyl)imidazolidin-1-yl]methyl butanoate
Inchi: InChI=1S/C20H20N2O4/c1-2-9-17(23)26-14-22-18(24)20(21-19(22)25,15-10-5-3-6-11-15
InchiKey: UPQWMVAELITTGQ-UHFFFAOYSA-N
Formula: C20H20N2O4
SMILES: CCCC(=O)OCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]: 352.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Aqueous Solubility Prediction Method
log10ws	-5.07		Estimated Solubility Method
logp	2.783		Crippen Method
mcvol	264.820	ml/mol	McGowan Method
tf	404.25	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