

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/ci9903071
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

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