

3-Ethanoxyloxymethylphenytoin

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/AqueousDataset002.xlsx
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/ci9903071

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/105-973-5/3-Ethanoyloxymethylphenytoin.pdf>

Generated by Cheméo on 2024-05-05 03:05:13.589316994 +0000 UTC m=+17167562.509894305.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.