

3-Heptanoyloxymethylphenytoin

Inchi:	InChI=1S/C23H26N2O4/c1-2-3-4-11-16-20(26)29-17-25-21(27)23(24-22(25)28,18-12-7-5
InchiKey:	FFGKFDRZZAJYCH-UHFFFAOYSA-N
Formula:	C23H26N2O4
SMILES:	CCCCCCC(=O)OCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]:	394.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.30		Estimated Solubility Method
logp	3.953		Crippen Method
mcvol	307.090	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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