

# 3-Hexanoyloxymethylphenyltoin

<b>Inchi:</b>	InChI=1S/C22H24N2O4/c1-2-3-6-15-19(25)28-16-24-20(26)22(23-21(24)27,17-11-7-4-8-
<b>InchiKey:</b>	OLWXRKNZPGNRLT-UHFFFAOYSA-N
<b>Formula:</b>	C22H24N2O4
<b>SMILES:</b>	CCCCCC(=O)OCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
<b>Mol. weight [g/mol]:</b>	380.44

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.89		Estimated Solubility Method
logp	3.563		Crippen Method
mcvol	293.000	ml/mol	McGowan Method

## Sources

<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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