3-Hexanoyloxymethylphenyltoin

Inchi: 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-
InchiKey: OLWXRKNZPGNRLT-UHFFFAOYSA-N
Formula: C22H24N2O4
SMILES: CCCCCC(=O)OCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O
Mol. weight [g/mol]: 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

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