

# 3,3-dimethyl-7-oxo-6-[(2-phenylacetyl)amino]-4-thia-

**Inchi:**  
**acid**

InChI=1S/C16H18N2O4S/c1-16(2)12(15(21)22)18-13(20)11(14(18)23-16)17-10(19)8-9-6

**InchiKey:**

JGSARLDLIJGVTE-UHFFFAOYSA-N

**Formula:**

C16H18N2O4S

**SMILES:**

CC1(C)SC2C(NC(=O)Cc3ccccc3)C(=O)N2C1C(=O)O

**Mol. weight [g/mol]:**

334.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Aqueous Solubility Prediction Method
logp	0.861		Crippen Method
mcvol	237.710	ml/mol	McGowan Method

## Sources

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Aqueous Solubility Prediction Method:**

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

**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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