

3,3-dimethyl-7-oxo-6-[[2-(phenoxy)acetyl]amino]-4-

Inchi:
acid

InChI=1S/C16H18N2O5S/c1-16(2)12(15(21)22)18-13(20)11(14(18)24-16)17-10(19)8-23

InchiKey:

BPLBGHOLXOTWMN-UHFFFAOYSA-N

Formula:

C16H18N2O5S

SMILES:

CC1(C)SC2C(NC(=O)COc3ccccc3)C(=O)N2C1C(=O)O

Mol. weight [g/mol]:

350.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Aqueous Solubility Prediction Method
logp	0.697		Crippen Method
mcvol	243.580	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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