

# 3-(3,5-Dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3.1.0]

<b>Inchi:</b>	InChI=1S/C13H11Cl2NO2/c1-12-6-13(12,2)11(18)16(10(12)17)9-4-7(14)3-8(15)5-9/h3-5
<b>InchiKey:</b>	QXJKBPAVAHBARF-UHFFFAOYSA-N
<b>Formula:</b>	C13H11Cl2NO2
<b>SMILES:</b>	CC12CC1(C)C(=O)N(c1cc(Cl)cc(Cl)c1)C2=O
<b>Mol. weight [g/mol]:</b>	284.14

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.80		Aqueous Solubility Prediction Method
logp	3.283		Crippen Method
mcvol	186.150	ml/mol	McGowan Method

## Sources

<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>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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