3-(3,5-Dichlorophenyl)-1,5-dimethyl-3-azabicyclo[3

Inchi: 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
InchiKey: QXJKBPAVAHBARF-UHFFFAOYSA-N
Formula: C13H11Cl2NO2
SMILES: CC12CC1(C)C(=O)N(c1cc(Cl)cc(Cl)c1)C2=O
Mol. weight [g/mol]: 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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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