

# amantadine

**Inchi:** InChI=1S/C15H12ClNO2/c1-8(15(18)19)9-2-4-11-12-7-10(16)3-5-13(12)17-14(11)6-9/h2  
**InchiKey:** PUXBGTOOZJQSKH-UHFFFAOYSA-N  
**Formula:** C15H12ClNO2  
**SMILES:** CC(C(=O)O)c1ccc2c(c1)[nH]c1ccc(Cl)cc12  
**Mol. weight [g/mol]:** 273.72

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Aqueous Solubility Prediction Method
logp	3.681		Crippen Method
mcvol	193.490	ml/mol	McGowan Method
tf	470.65	K	Aqueous Solubility Prediction 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/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  
**tf:** Normal melting (fusion) point

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