

# nitrofurantoin

**Inchi:** InChI=1S/C18H20FN3O4/c1-10-9-26-17-14-11(16(23)12(18(24)25)8-22(10)14)7-13(19)1  
**InchiKey:** GSDSWSVVBLHKDQ-UHFFFAOYSA-N  
**Formula:** C18H20FN3O4  
**SMILES:** CC1COc2c(N3CCN(C)CC3)c(F)cc3c(=O)c(C(=O)O)cn1c23  
**Mol. weight [g/mol]:** 361.37

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Aqueous Solubility Prediction Method
logp	1.544		Crippen Method
mcvol	250.430	ml/mol	McGowan Method
tf	526.65	K	Aqueous Solubility Prediction Method

## Sources

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

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

## 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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