

# Isbufylline

<b>Inchi:</b>	InChI=1S/C11H16N4O2/c1-7(2)5-15-6-12-9-8(15)10(16)14(4)11(17)13(9)3/h6-7H,5H2,1-
<b>InchiKey:</b>	WHUWQSQEVISUMC-UHFFFAOYSA-N
<b>Formula:</b>	C11H16N4O2
<b>SMILES:</b>	CC(C)Cn1cnc2c1c(=O)n(C)c(=O)n2C
<b>Mol. weight [g/mol]:</b>	236.28

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.090		Crippen Method
mcvol	178.590	ml/mol	McGowan Method

## Sources

**Aqueous and cosolvent solubility data for drug-like organic compounds:** <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/>  
**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

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