

# 1-[[4-(1,3-benzothiazol-2-yl)phenyl]methyl-ethoxyphosphoryl]pyrrolidin-2-one

<b>Inchi:</b>	InChI=1S/C20H21N2O3PS/c1-2-25-26(24,22-13-5-8-19(22)23)14-15-9-11-16(12-10-15)2
<b>InchiKey:</b>	HTAUUADKDLLMRU-UHFFFAOYSA-N
<b>Formula:</b>	C20H21N2O3PS
<b>SMILES:</b>	CCOP(=O)(Cc1ccc(-c2nc3ccccc3s2)cc1)N1CCCC1=O
<b>Mol. weight [g/mol]:</b>	400.44

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Aqueous Solubility Prediction Method
logp	5.315		Crippen Method
mcvol	289.200	ml/mol	McGowan Method

## Sources

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