

3-hydroxy-2-methyl-1-phenylpyridin-4-one

Inchi:	InChI=1S/C12H11NO2/c1-9-12(15)11(14)7-8-13(9)10-5-3-2-4-6-10/h2-8,15H,1H3
InchiKey:	BNXSABDYGOUQQI-UHFFFAOYSA-N
Formula:	C12H11NO2
SMILES:	<chem>Cc1c(O)c(=O)ccn1-c1ccccc1</chem>
Mol. weight [g/mol]:	201.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Aqueous Solubility Prediction Method
logp	1.852		Crippen Method
mcvol	154.140	ml/mol	McGowan Method

Sources

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

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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