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: Cc1c(O)c(=O)ccn1-c1ccccc1
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/AqueousDa
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