3-hydroxy-2-methyl-1-(4-methylphenyl)pyridin-4-c

Inchi: InChI=1S/C13H13NO2/c1-9-3-5-11(6-4-9)14-8-7-12(15)13(16)10(14)2/h3-8,16H,1-2H3
InchiKey: YKWMYPVOGWWSKR-UHFFFAOYSA-N
Formula: C13H13NO2
SMILES: Cc1ccc(-n2ccc(=O)c(O)c2C)cc1
Mol. weight [g/mol]: 215.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Aqueous Solubility Prediction Method
logp	2.160		Crippen Method
mcvol	168.230	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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

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