pyridoxal 5-phosphate

Other names: (4-formyl-5-hydroxy-6-methylpyridin-3-yl)methyl dihydrogen phosphate
Inchi: InChI=1S/C8H10NO6P/c1-5-8(11)7(3-10)6(2-9-5)4-15-16(12,13)14/h2-3,11H,4H2,1H3,(H
InchiKey: NGVDGCNFYWLIFO-UHFFFAOYSA-N
Formula: C8H10NO6P
SMILES: Cc1ncc(COP(=O)(O)O)c(C=O)c1O
Mol. weight [g/mol]: 247.14

Physical Properties

Property code	Value	Unit	Source
logp	0.517		Crippen Method
mcvol	161.180	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

Solubility Determination and Correlation for Pyridoxal 5-Phosphate Monohydrate in Different Binary Solvents from 278.15 K to 318.15 K: https://www.doi.org/10.1021/acs.jced.8b00309
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume