

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:	NGVDGCNFWLIFO-UHFFFAOYSA-N
Formula:	C8H10NO6P
SMILES:	<chem>Cc1ncc(COP(=O)(O)O)c(C=O)c1O</chem>
Mol. weight [g/mol]:	247.14

Physical Properties

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

Sources

Cheméo Relay (1.0, beta):

Solubility Determination and Correlation for Pyridoxal 5-Phosphate Monophosphate in Different Binary Solvents from 278.15 K to 318.15 K: Crippen Method:

<https://www.doi.org/10.1021/acs.jced.8b00309>

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

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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

Latest version available from:

<https://www.chemeo.com/cid/107-483-7/pyridoxal-5-phosphate.pdf>

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