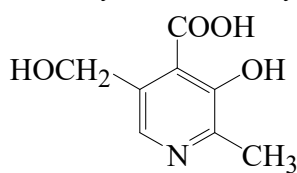




>>Entry Name: 3-Hydroxy-5-(hydroxymethyl)-2-methyl-4-pyridinecarboxylic acid, 9Cl

Synonym(s): 3-Hydroxy-5-(hydroxymethyl)-2-methylisonicotinic acid, 8Cl. 4-Pyridoxinecarboxylic acid. Pyridoxinic acid. Pyridoxylic acid. Pyridoxic acid



CAS Registry Number: 82-82-6

Molecular Formula: C₈H₉NO₄

Molecular Weight: 183.163

Accurate Mass: 183.053159

Percentage Composition: C 52.46%; H 4.95%; N 7.65%; O 34.94%

Biological Source: Isol. from human urine

Metabolism: Oxidative metab. of Pyridoxine [BDV40-Q](#) and Pyridoxamine [GCG13-J](#)

Physical Description: Wedge-shaped cryst. (Py)

Melting Point: Mp 247-248°. Mp 258-261° (dec.)

Solubility: Sl. sol. H₂O, EtOH, Py ; insol. Et₂O, aq. acid soln.; v. sol. aq. alk. soln.

pKa Value: pK_{a1} 5.5 (carboxyl group); pK_{a2} 9.75 (phenolic group)

Other Data: Excreted in urine and sweat. Displays characteristic blue fluor. (max at pH 3-4)

>>Derivative: Lactone

Synonym(s): 7-Hydroxy-6-methyl-furo[3,4-*c*]pyridin-1(3*H*)-one, 9Cl, 8Cl. β-Pyracin. 4-Pyridoxolactone

Extra CAS Registry Numbers(s): 4753-19-9

Molecular Formula: C₈H₇NO₃

Molecular Weight: 165.148

Accurate Mass: 165.042594

Percentage Composition: C 58.18%; H 4.27%; N 8.48%; O 29.06%

Physical Description: Light yellow prismatic cryst. (EtOH aq.)

Melting Point: Mp 263-265°

References:

Huff, J.W. *et al.*, *J. Biol. Chem.*, 1944, **155**, 345-355, (*isol, metab, synth, props, lactone*)

Johnson, B.C. *et al.*, *J. Biol. Chem.*, 1945, **158**, 619-623, (*metab, occur*)

Chrisley, B. Mc., *J. Chromatogr.*, 1991, **563**, 369-378, (*anal, hplc*)

Japan. Pat., 1992, 04 95 074; *CA*, **117**, 90051d, (*synth*)

Merck Index, 12th edn., 1996, No. 8165, (*props*)