



Formula: C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>

MW: 179.22

CAS: 536-69-6

MDL: MFCD00006298

TNP: TNP00268

FUSARIC ACID; FURASIC ACID; 5-N-BUTYL-2-PICOLINIC ACID; 5-N-BUTYLPICOLINIC ACID; 5-BUTYL-2-PYRIDINECARBOXYLIC ACID; 5-BUTYLPICOLINIC ACID; 5-BUTYLPYRIDINE-2-CARBOXYLIC ACID; 5-butyl-2-pyridinecarboxylicaci



LogP: 2.45

LogS:

Acceptors: 2

Donors: 1

Rotation Bonds: 5

Chiral Centers: 0

N+O: 3

LIPINSKY: 4

IUPAC: 5-butylpyridine-2-carboxylic acid

Smiles: n1c(C(=O)O)ccc(c1)CCCC

Physiol Action: Inhibits dopamine beta-hydroxylase activity

THERAPEUTIC CATEGORY: Antibiotic

REFERENCE: Wang, H. and Ng, T.B., Pharmacological activities of fusaric acid (5-butylpicolinic acid). Life Sci. 65, 849, (1999) abstract Bencsics, A., et al., Dopamine, as well as norepinephrine, is a link between noradrenergic nerve terminals and splenocytes. Brain Res. 761, 236-243, (1997) abstract Baillien, M., et al., Regional distribution and control of tyrosine hydroxylase activity in the quail brain. Brain Res. Bull. 48, 31-37, (1999) abstract Merck Merck 13,4335

SOURCE: Fusaric acid from *Gibberella fujikuroi*

ACTIVITY: Dopamine beta-hydroxylase inhibitor

Specification: FUSARIC ACID Chemical Properties:

mp 96-100 C storage temp. -20C solubility ethanol: 50 mg/mL, clear, faintly yellow Merck 4314 CAS DataBase Reference 536-69-6 (CAS DataBase Reference) Safety Information Hazard Codes Xn Risk Statements 22 Safety Statements 24/25 RIDADR 2811 WGK Germany 3 RTECS US5625000 F 10 Hazard Class 6.1(b) Packing Group III FUSARIC ACID Usage And Synthesis Chemical Properties:

off-white to faint yellowish crystalline powder FUSARIC ACID Raw materials Ethanol-->Hydrochloric acid-->Diethyl ether-->Sulfuric acid -->Dichloromethane-->Sodium carbonate-->Chloroform-->Magnesium sulfate-->Potassium hydroxide -->Triethylamine-->Sodium chloride-->Acetonitrile-->1,4-Dioxane-->Formaldehyde-->Trisodium phosphate dodecahydrate-->Dimethylamine hydrochloride-->Caproaldehyde-->1,1-Dimethylhydrazine-->2-Chloroacrylonitrile

Merck 13 Reference: Monograph Number: 0004335

Title: Fusaric Acid

CAS Registry Number: 536-69-6

CAS Name: 5-Butyl-2-pyridinecarboxylic acid

Additional Names: 5-butylpicolinic acid

Molecular Formula: C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>

Molecular Weight: 179.22.

Percent Composition: C 67.02%, H 7.31%, N 7.82%, O 17.85%

Literature References: Antibiotic (wilting agent) first isolated from the fungus *Fusarium*

heterosporium, Nees: Yabuta et al., J. Agric. Chem. Soc. Jpn. 10, 1059 (1934). Isolation from other *Fusarium* species and from *Gibberella fujikuroi* and synthesis: Plattner et al., *Helv. Chim. Acta* 37, 1379 (1954). Prepn: Hardegger, Nikles, *ibid.* 39, 505 (1956); 40, 2428 (1957); Schreiber, Adam, *Ber.* 93, 1848 (1960); Umezawa, Nagatsu, DE 2005255 (1970 to *Microbiochem. Res. Found.*); R. Tschesche, W. F