



Formula: C<sub>10</sub>H<sub>7</sub>NO<sub>3</sub>

MW: 189.17

CAS: 492-27-3

TNP NUMBER: TNP00449

MDL NUMBER: MFCD00006753

IUPAC: 4-hydroxyquinoline-2-carboxylic acid

Smiles: n1c(cc(c2c1cccc2)O)C(=O)O

ACCEPTORS: 3

DONORS: 2

ROTATION BONDS: 3

N+O: 4

Chiral Centers: 0

LogP: 1.25

LogS: -2.9

LIPINSKI: 4

Monograph Number: 0005342

Title: Kynurenic Acid

CAS Registry Number: 492-27-3

CAS Name: 4-Hydroxy-2-quinolinecarboxylic acid

Additional Names: 4-hydroxyquinaldic acid

Molecular Formula: C<sub>10</sub>H<sub>7</sub>NO<sub>3</sub>

Molecular Weight: 189.17.

Percent Composition: C 63.49%, H 3.73%, N 7.40%, O 25.37%

Literature References: Found in the urine of some animals as a metabolic product of tryptophan; its excretion is stepped up in avitaminoses B<sub>1</sub>, B<sub>2</sub> and B<sub>6</sub>. Isoln and syntheses: Spath, *Monatsh. Chem.* 42, 89 (1921); Besthorn, *Ber.* 54, 1330 (1921). Alternate syntheses: Benassi, *Gazz. Chim. Ital.* 91, 1097 (1961); Wald, Joullie, *J. Org. Chem.* 31, 3369 (1966); Jordanides, *Ann.* 729, 244 (1969).

Properties: Yellow needles, mp 282-283. Soly in water: about 0.9% at 100. Sol in hot alc. Insol in ether.

Melting point: mp 282-283

Derivative Type: Methyl ester

Molecular Formula: C<sub>11</sub>H<sub>9</sub>NO<sub>3</sub>

Molecular Weight: 203.19.

Percent Composition: C 65.02%, H 4.46%, N 6.89%, O 23.62%

Properties: Yellow crystals, mp 224. Cf. xanthurenic acid.

Melting point: mp 224

Use: In nutrition studies, specifically in vitamin B deficiency diseases.

Synonyms: T Acid/ 1-Naphthylamine-3,6-8-Trisulfonic Acid

CAS:

MF:

MW:0

EINECS:

Product Categories: T Acid/ 1-Naphthylamine-3,6-8-Trisulfonic Acid T Acid/  
1-Naphthylamine-3,6-8-Trisulfonic Acid

Usage And Synthesis: T Acid/ 1-Naphthylamine-3,6-8-Trisulfonic Acid

