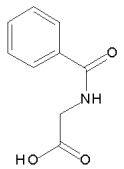

Formula: C9H9NO3

MW: 179.18

CAS: 495-69-2

MDL: MFCD00002692

TNP: TNP00451

BENZAMINOACETIC ACID; BENZOYLAMINOACETIC ACID; BENZOYLGLYCINE; BZ-GLY-OH; BZO-GLY-OH; HIPPURIC ACID; AKOS B029712; TIMTEC-BB SBB003759

LogP: -3.29

LogS: -1.73

Acceptors: 3

Donors: 2

Rotation Bonds: 3

Chiral Centers: 0

N+O: 4

LIPINSKY: 4

Info: Present in urine of herbivorous animals; also in smaller amounts in human urine

IUPAC: 2-(phenylcarbonylamino)acetic acid

Smiles: C(NCC(=O)O)(=O)c1ccccc1

Specification: Intermediates of Dyes and Pigments; Aromatic Cinnamic Acids, Esters and

Derivatives HIPPURIC ACID Chemical Properties:

 mp 187-191 C(lit.) density 1,371 g/cm3 storage temp. Store at RT. Merck 14,4716 BRN 1073987 Stability:Stable. Incompatible with oxidizing agents. CAS DataBase Reference495-69-2(CAS DataBase Reference) Safety Information Hazard Codes Xn,Xi Risk Statements 22-37/38-41-36/37/38 Safety Statements 26-39-36/37-22 WGK Germany 3 RTECS MR8150000 F 3-10 HazardClass IRRITANT HIPPURIC ACID Usage And Synthesis Chemical Properties:

White crystalline powder HIPPURIC ACID Preparation ProductsBenzoic acid-->DOPAC-->(3,4-Dimethoxyphenyl)acetic acid-->DL-Isoleucine-->2-BENZAMIDO-3-(4-(N,N-BIS-(2-CHLOROETHYL)AMINO)PHENYL)PROPIONIC ACID-->DL-3-(4-Fluorophenyl)alanine Raw materialsGlycine-->Benzoyl chloride-->SODIUM GLYCINATE

Merck 13 Reference: Monograph Number: 0004735

Title: Hippuric Acid

CAS Registry Number: 495-69-2

CAS Name: N-Benzoylglycine

Additional Names: benzoylaminoacetic acid; benzamidoacetic acid

Molecular Formula: C9H9NO3

Molecular Weight: 179.17.

Percent Composition: C 60.33%, H 5.06%, N 7.82%, O 26.79%

Line Formula: C6H5CONHCH2COOH

Literature References: Present in the urine of herbivorous animals; also in smaller amounts in human urine. Prepd from benzoyl chloride and glycine in NaOH soln: Ingersoll, Babcock, Org. Synth. coll. vol. II, 328 (1943).

Properties: Crystals. mp 187-188. One gram dissolves in about 250 ml cold water, 1000 ml chloroform, 400 ml ether, 60 ml amyl alcohol; slightly sol in cold, freely in hot alcohol or hot water; also sol in aq soln of sodium phosphate. Practically insol in benzene, carbon disulfide, petr ether.

Melting point: mp 187-188

Derivative Type: Ammonium salt

Molecular Formula: $NH_4C_9H_8NO_3$

Molecular Weight: 196.20.

Percent Composition: N 14.28%, H 6.16%, C 55.09%, O 24.46%

Properties: Crystals. Freely sol in water; sol in alcohol.

Derivative Type: Potassium salt monohydrate

Molecular Formula: $KC_9H_{10}NO_4.H_2O$

Molecular Weight: 253.29.

Percent Composition: K 15.44%, C 42.68%, H 4.78%, N 5.53%, O 31.58%

Properties: Cryst powder. Very sol in water; sol in alcohol.