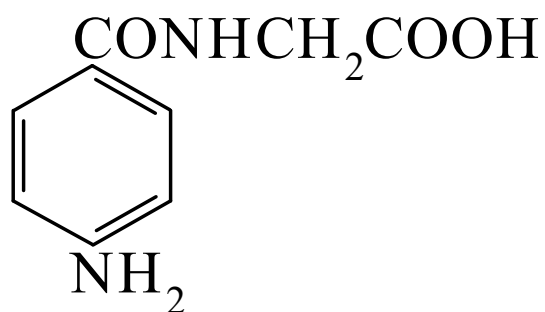




>>Entry Name: *N*-(4-Aminobenzoyl)glycine, 9CI

Synonym(s): Aminohippuric acid, USAN. (4-Aminobenzoyl)aminoacetic acid. Nefrotest. Nephrotest. Renotest. PAHA



CAS Registry Number: 61-78-9

Related CAS Registry Numbers(s): 94-16-6

Molecular Formula: $\text{C}_9\text{H}_{10}\text{N}_2\text{O}_3$

Molecular Weight: 194.19

Accurate Mass: 194.069143

Percentage Composition: C 55.67%; H 5.19%; N 14.43%; O 24.72%

Use/Importance: Diagnostic aid (renal function detn.)

Physical Description: Needles (H_2O)

Melting Point: Mp 198-199°

Calculated Log P Data: Log P -0.28 (calc)

Aldrich: 12295-5

Fluka: 8090

Sigma: A1422

>>Derivative: Na salt

Synonym(s): Aminohippurate sodium, USAN

CAS Registry Number: 94-16-6

Physical Description: Cryst.

Melting Point: Mp 123-125° (hydrate)

Other Data: CAS no. refers to the monohydrate

Hazard & Toxicity: LD₅₀ (rat, ivn) 4075 mg/kg

Sigma: A3759

>>Derivative: Me ester

CAS Registry Number: 5259-86-9

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_3$

Molecular Weight: 208.216

Accurate Mass: 208.084793

Percentage Composition: C 57.69%; H 5.81%; N 13.45%; O 23.05%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 130-131°

>>Derivative: Et ester

CAS Registry Number: 20333-85-1

Molecular Formula: $\text{C}_{11}\text{H}_{14}\text{N}_2\text{O}_3$

Molecular Weight: 222.243

Accurate Mass: 222.100443

Percentage Composition: C 59.45%; H 6.35%; N 12.60%; O 21.60%

Physical Description: Cryst. (H_2O)

Melting Point: Mp 94-95°

>>Derivative: Amide

Molecular Formula: $\text{C}_9\text{H}_{11}\text{N}_3\text{O}_2$

Molecular Weight: 193.205

Accurate Mass: 193.085127

Percentage Composition: C 55.95%; H 5.74%; N 21.75%; O 16.56%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 228° (dec.) (225 - 226°)

References: