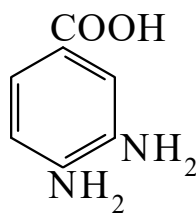




>>Entry Name: 3,4-Diaminobenzoic acid, 9CI



CAS Registry Number: 619-05-6

Molecular Formula: C₇H₈N₂O₂

Molecular Weight: 152.152

Accurate Mass: 152.058578

Percentage Composition: C 55.26%; H 5.30%; N 18.41%; O 21.03%

Use/Importance: Used as 0.6% aq. DMF or 0.1M HCl soln. for photometric detn. of Ru ($\lambda_{\max}$ 550 nm, ϵ 4200), Pt ($\lambda_{\max}$ 715 nm, ϵ 11400). Can be homopolym. to a poly(benzimidazole)

Physical Description: Leaflets

Melting Point: Mp 207°. Mp 210-211 dec.°. Mp 215-218°

Solubility: Sl. sol. H₂O; sol. DMF, acids

pKa Value: pK_a 7.77 (80% 2-methoxyethanol)

Aldrich: D1260-0

Fluka: 32760

Sigma: D3391

>>Derivative: Me ester

CAS Registry Number: 36692-49-6

Molecular Formula: C₈H₁₀N₂O₂

Molecular Weight: 166.179

Accurate Mass: 166.074228

Percentage Composition: C 57.82%; H 6.07%; N 16.86%; O 19.26%

Physical Description: Needles (H₂O)

Melting Point: Mp 108-109°

>>Derivative: Et ester

CAS Registry Number: 37466-90-3

Molecular Formula: C₉H₁₂N₂O₂

Molecular Weight: 180.206

Accurate Mass: 180.089878

Percentage Composition: C 59.99%; H 6.71%; N 15.55%; O 17.76%

Physical Description: Needles (H₂O)

Melting Point: Mp 112-113°

>>Derivative: Nitrile

Synonym(s): 3,4-Diaminobenzonitrile, 9CI. 4-Cyano-1,2-benzenediamine

CAS Registry Number: 17626-40-3

Molecular Formula: C₇H₇N₃

Molecular Weight: 133.152

Accurate Mass: 133.063997

Percentage Composition: C 63.14%; H 5.30%; N 31.56%

Physical Description: Brown solid

Melting Point: Mp 144-146°

>>Derivative: 4-*N*-Ac, Me ester

Molecular Formula: C₁₀H₁₂N₂O₃

Molecular Weight: 208.216

Accurate Mass: 208.084793

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

Physical Description: Solid (EtOH/Et₂O)

Melting Point: Mp 187-190°