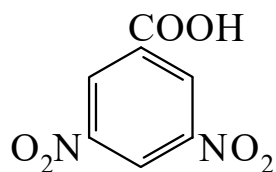




>>Entry Name: 3,5-Dinitrobenzoic acid, 9CI, 8CI



CAS Registry Number: 99-34-3

Type of Compound Code(s): PG5100

Molecular Formula: C₇H₄N₂O₆

Molecular Weight: 212.118

Accurate Mass: 212.006938

Percentage Composition: C 39.64%; H 1.90%; N 13.21%; O 45.26%

Use/Importance: Corrosion inhibitor, also used in photography. Can be used to identify the alcohol components in esters. Used as a fluometric assay for creatinine

Physical Description: Yellow or colourless cryst. (dimorph.)

Melting Point: Mp 212-213°

pKa Value: pK_a 2.82 (25°, H₂O)

Aldrich: 12125-8

Fluka: 41950

Sigma: D4766

>>Derivative: Me ester

CAS Registry Number: 2702-58-1

Molecular Formula: C₈H₆N₂O₆

Molecular Weight: 226.145

Accurate Mass: 226.022588

Percentage Composition: C 42.49%; H 2.67%; N 12.39%; O 42.45%

Melting Point: Mp 112°

Aldrich: 38636-7

>>Derivative: Et ester

CAS Registry Number: 618-71-3

Molecular Formula: C₉H₈N₂O₆

Molecular Weight: 240.172

Accurate Mass: 240.038238

Percentage Composition: C 45.01%; H 3.36%; N 11.66%; O 39.97%

Melting Point: Mp 93°

Aldrich: 30133-7

>>Derivative: Chloride

CAS Registry Number: 99-33-2

Type of Compound Code(s): PG5250 PG5100

Molecular Formula: C₇H₃ClN₂O₅

Molecular Weight: 230.564

Accurate Mass: 229.97305

Percentage Composition: C 36.47%; H 1.31%; Cl 15.38%; N 12.15%; O 34.70%

Use/Importance: Reagent for isol. and characterisation of alcohols and amines

Physical Description: Needles

Melting Point: Mp 74°

Boiling Point: Bp₁₁ 196°

Hazard & Toxicity: Irritant

Aldrich: 15627-2

Fluka: 42030

Sigma: D4386