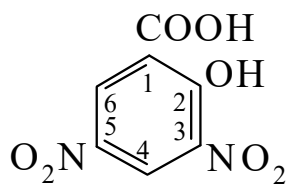




>>Entry Name: 2-Hydroxy-3,5-dinitrobenzoic acid

Synonym(s): 3,5-Dinitrosalicylic acid



CAS Registry Number: 609-99-4

Related CAS Registry Numbers(s): 46506-88-1

Molecular Formula: C₇H₄N₂O₇

Molecular Weight: 228.118

Accurate Mass: 228.001853

Percentage Composition: C 36.86%; H 1.77%; N 12.28%; O 49.10%

Use/Importance: Reagent for spectrophotometric anal. of reducing sugars. Derivatisation reagent for the chromatog. sepn. of unsymmetric hydrazines. Shows extensive complexing behaviour

Physical Description: Plates + 1H₂O (H₂O)

Melting Point: Mp 173-174°

pKa Value: pK_{a1} 0.45; pK_{a2} 7.4 (25°, 0.1M KNO₃)

Aldrich: 12884-8

Fluka: 42260

Sigma: D0550

>>Derivative: Me ester

CAS Registry Number: 22633-33-6

Molecular Formula: C₈H₆N₂O₇

Molecular Weight: 242.145

Accurate Mass: 242.017503

Percentage Composition: C 39.68%; H 2.50%; N 11.57%; O 46.25%

Melting Point: Mp 127-128°

Aldrich: 40717-8

Sigma: D7294

>>Derivative: Et ester

CAS Registry Number: 22557-74-0

Molecular Formula: C₉H₈N₂O₇

Molecular Weight: 256.171

Accurate Mass: 256.033153

Percentage Composition: C 42.20%; H 3.15%; N 10.94%; O 43.72%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 99°

>>Derivative: Ph ester

CAS Registry Number: 52040-46-7

Molecular Formula: C₁₃H₈N₂O₇

Molecular Weight: 304.215

Accurate Mass: 304.033153

Percentage Composition: C 51.33%; H 2.65%; N 9.21%; O 36.81%

Physical Description: Cryst.

Melting Point: Mp 183°

>>Derivative: Amide

CAS Registry Number: 2912-79-0

Molecular Formula: C₇H₅N₃O₆

Molecular Weight: 227.133

Accurate Mass: 227.017837

Percentage Composition: C 37.02%; H 2.22%; N 18.50%; O 42.26%

Physical Description: Yellow cryst. (H₂O)

Melting Point: Mp 181°