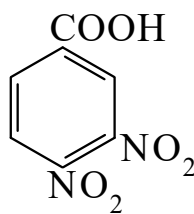




>>Entry Name: 3,4-Dinitrobenzoic acid, 9Cl, 8Cl



CAS Registry Number: 528-45-0

Type of Compound Code(s): PG5350

Molecular Formula: $C_7H_4N_2O_6$

Molecular Weight: 212.118

Accurate Mass: 212.006938

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

Use/Importance: Reagent for microdetn. of sugar components in polysaccharide hydrolysates

Melting Point: Mp 165°

pKa Value: pK_a 2.82 (25°, H₂O)

>>Derivative: Me ester

CAS Registry Number: 22907-68-2

Molecular Formula: $C_8H_6N_2O_6$

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 87°

>>Derivative: Et ester

CAS Registry Number: 35998-99-3

Molecular Formula: $C_9H_8N_2O_6$

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 71°

>>Derivative: Chloride

CAS Registry Number: 24376-18-9

Molecular Formula: $C_7H_3ClN_2O_5$

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%

Melting Point: Mp 50-51°

Boiling Point: Bp₁₇ 188°

>>Derivative: Amide

Molecular Formula: $C_7H_5N_3O_5$

Molecular Weight: 211.134

Accurate Mass: 211.022922

Percentage Composition: C 39.82%; H 2.39%; N 19.90%; O 37.89%

Melting Point: Mp 165-166°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-1,2-dinitrobenzene

CAS Registry Number: 4248-33-3

Molecular Formula: $C_7H_3N_3O_4$

Molecular Weight: 193.118

Accurate Mass: 193.012357

Percentage Composition: C 43.54%; H 1.57%; N 21.76%; O 33.14%

Melting Point: Mp 90-92°

References: