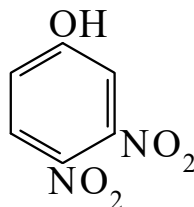




>>Entry Name: 3,4-Dinitrophenol

Synonym(s): δ -Dinitrophenol



CAS Registry Number: 577-71-9

Extra CAS Registry Numbers(s): 25550-58-7

Type of Compound Code(s): PA5000 PS7750 PS7850

Molecular Formula: $C_6H_4N_2O_5$

Molecular Weight: 184.108

Accurate Mass: 184.012023

Percentage Composition: C 39.14%; H 2.19%; N 15.22%; O 43.45%

Use/Importance: Used as EtOH soln. in gravimetric detn. of Zr; acid base indicator

Physical Description: Yellowish needles (H_2O)

Melting Point: Mp 134°

Solubility: Sol. EtOH, Et_2O ; sl. sol. H_2O

pKa Value: pK_a 5.42 (25°)

Hazard & Toxicity: Potentially explosive. May cause dermatitis. LD_{50} (rat, ipr) 98 mg/kg

Fluka: 42195

Supelco: R42-8490

>>Derivative: Me ether

Synonym(s): 4-Methoxy-1,2-dinitrobenzene, 9Cl. 3,4-Dinitroanisole, 8Cl

CAS Registry Number: 4280-28-8

Molecular Formula: $C_7H_6N_2O_5$

Molecular Weight: 198.135

Accurate Mass: 198.027673

Percentage Composition: C 42.43%; H 3.05%; N 14.14%; O 40.38%

Physical Description: Yellow needles

Melting Point: Mp 70°

>>Derivative: Et ether

Synonym(s): 4-Ethoxy-1,2-dinitrobenzene. 3,4-Dinitrophenetole

Molecular Formula: $C_8H_8N_2O_5$

Molecular Weight: 212.162

Accurate Mass: 212.043323

Percentage Composition: C 45.29%; H 3.80%; N 13.20%; O 37.71%

Melting Point: Mp 87°

References:

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Bishop, E., *Indicators*, Pergamon, Oxford, 1972, (*indicator*)

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