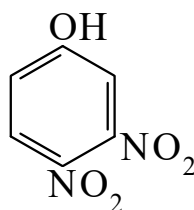




>>Entry Name: 3,4-Dinitrophenol

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: C₆H₄N₂O₅

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 (H₂O)

Melting Point: Mp 134°

Solubility: Sol. EtOH, Et₂O; sl. sol. H₂O

pKa Value: pK_a 5.42 (25°)

Hazard & Toxicity: Potentially explosive. May cause dermatitis. LD₅₀ (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: C₇H₆N₂O₅

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: C₈H₈N₂O₅

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:

Vermeulen, H., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1906, **25**, 12-31, (*Me ether*)

Granzhan, V.A. *et al.*, *CA*, 1972, **77**, 19290, (*synth*)

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

Di Nunno, L. *et al.*, *J.C.S. Perkin I*, 1973, 1954-1955, (*deriv*)

Hazards in the Chemical Laboratory, 3rd edn., (ed. Bretherick, L.), Royal Society of Chemistry, 1981, 310

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DVA400