



>>Entry Name: 2,4-Dinitrophenol

Synonym(s): α -Dinitrophenol

CAS Registry Number: 51-28-5

Related CAS Registry Numbers(s): 1011-73-0

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

Type of Compound Code(s): PS8300 PS7850 PS7750 PA5000 PA4200

Structure by analogy with 2,3-Dinitrophenol, [FBF50-V](#)

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 for gravimetric detn. of Zr; indirect photometric detn. of $SO_4^{2(-)}$; as acid-base indicator. Oxidative phosphorylation uncoupler

Physical Description: Yellow plates (H_2O)

Melting Point: Mp 113°. Mp 106-108°

Solubility: Sol. EtOH, Me_2CO , C_6H_6 ; sl. sol. H_2O

pKa Value: pK_a 4 (25°)

Other Data: Sublimes. Steam-volatile

Hazard & Toxicity: Forms explosive salts with alkalis or NH_3 . V. toxic if swallowed. Readily absorbed through skin. Can cause dermatitis, cataracts, weight loss, granulocytopenia and polyneuropathy. Other symptoms of human exposure recorded. LD_{50} (rat, orl) 30 mg/kg. Exp. reprod. and teratogenic effects

Aldrich: D19850-1

Fluka: 42170

Sigma: D7004

Supelco: 4-8550

>>Derivative: Ac

CAS Registry Number: 4232-27-3

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 72°

>>Derivative: Benzoyl

CAS Registry Number: 1523-15-5

Molecular Formula: $C_{13}H_8N_2O_6$

Molecular Weight: 288.216

Accurate Mass: 288.038238

Percentage Composition: C 54.18%; H 2.80%; N 9.72%; O 33.31%

Melting Point: Mp 134-135°

>>Derivative: 4-Methylbenzenesulfonyl

Melting Point: Mp 122°

>>Derivative: Me ether

Synonym(s): 1-Methoxy-2,4-dinitrobenzene. 2,4-Dinitroanisole

CAS Registry Number: 119-27-7

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: Cryst. (EtOH)

Melting Point: Mp 83°

Hazard & Toxicity: Toxic, potentially explosive

Rare Chemicals Library: S62763-1