>>**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 alkalies 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