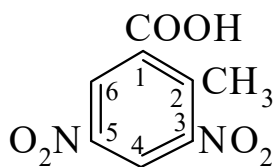




>>Entry Name: 2-Methyl-3,5-dinitrobenzoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3,5-Dinitro-*o*-toluic acid, 8CI. 4,6-Dinitro-*o*-toluic acid (incorr.)



CAS Registry Number: 28169-46-2

Molecular Formula: C₈H₆N₂O₆

Molecular Weight: 226.145

Accurate Mass: 226.022588

Percentage Composition: C 42.49%; H 2.67%; N 12.39%; O 42.45%

Physical Description: Needles (H₂O)

Melting Point: Mp 205-206°

Aldrich: 21142-7

>>Derivative: Me ester

CAS Registry Number: 52090-24-1

Molecular Formula: C₉H₈N₂O₆

Molecular Weight: 240.172

Accurate Mass: 240.038238

Percentage Composition: C 45.01%; H 3.36%; N 11.66%; O 39.97%

Physical Description: Needles (MeOH)

Melting Point: Mp 74-75°

Rare Chemicals Library: S30919-2

>>Derivative: Et ester

Molecular Formula: C₁₀H₁₀N₂O₆

Molecular Weight: 254.199

Accurate Mass: 254.053888

Percentage Composition: C 47.25%; H 3.97%; N 11.02%; O 37.76%

Melting Point: Mp 15°

Boiling Point: Bp₇₅₀ 204°

>>Derivative: Chloride

CAS Registry Number: 39614-85-2

Molecular Formula: C₈H₅ClN₂O₅

Molecular Weight: 244.591

Accurate Mass: 243.9887

Percentage Composition: C 39.29%; H 2.06%; Cl 14.49%; N 11.45%; O 32.71%

Physical Description: Needles (petrol)

Melting Point: Mp 68°

>>Derivative: Amide

Synonym(s): 2-Methyl-3,5-dinitrobenzamide, 9CI. **Dinitolmide**, BAN, INN. Abilene. Salcostat. Whitsyn T. Zamix. Zoalene. Zoamix

CAS Registry Number: 148-01-6

Molecular Formula: C₈H₇N₃O₅

Molecular Weight: 225.16

Accurate Mass: 225.038572

Percentage Composition: C 42.68%; H 3.13%; N 18.66%; O 35.53%

Use/Importance: Poultry feed additive. Coccidiostat

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 181°

Calculated Log P Data: Log P 0.63 (calc)

Hazard & Toxicity: Has exploded on drying in bulk. Dust explosion hazard. LD₅₀ (rat, orl) 600 mg/kg. ACGIH TLV: long-term 5 mg m⁻³

>>Derivative: Nitrile

Synonym(s): 1-Cyano-2-methyl-3,5-dinitrobenzene