



>>Entry Name: 4-Methyl-3,5-dinitrobenzoic acid, 9CI

Synonym(s): 3,5-Dinitro-*p*-toluic acid, 8CI. 2,6-Dinitro-*p*-toluic acid (incorr.)

CAS Registry Number: 16533-71-4

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: Yellow leaflets (H₂O)

Melting Point: Mp 160°

pK_a Value: pK_a 2.97 (25°, H₂O)

Other Data: Functions as a host accommodating guest molecules in cavities created by coupling of 6 neighbouring molecules through H-bonding

Aldrich: 13688-3

Fluka: 42130

>>Derivative: Me ester

CAS Registry Number: 49592-71-4

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 87-88°

>>Derivative: Et ester

CAS Registry Number: 5400-86-2

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%

Physical Description: Needles (EtOH)

Melting Point: Mp 75°

>>Derivative: Amide

CAS Registry Number: 4551-76-2

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%

Physical Description: Needles

Melting Point: Mp 187°

>>Derivative: Chloride

CAS Registry Number: 6633-28-9

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: Yellow platelets (petrol)

Melting Point: Mp 58°

References:

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Wheeler, A.S. *et al.*, *J.A.C.S.*, 1927, **49**, 494-499, (*synth*)

Brady, O.L. *et al.*, *J.C.S.*, 1934, 114-121, (*synth, esters*)

Barben, I.K. *et al.*, *J.C.S.*, 1960, 672-676, (*synth, amide*)

Buck, P. *et al.*, *Chem. Ber.*, 1970, **103**, 1420-1430, (*synth*)

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