



---

>>Entry Name: 2-Methyl-3,5-dinitroaniline

Synonym(s): 2-Methyl-3,5-dinitrobenzenamine, 9Cl. 3,5-Dinitro-*o*-toluidine

CAS Registry Number: 35572-78-2

Molecular Formula: C<sub>7</sub>H<sub>7</sub>N<sub>3</sub>O<sub>4</sub>

Molecular Weight: 197.15

Accurate Mass: 197.043657

Percentage Composition: C 42.65%; H 3.58%; N 21.31%; O 32.46%

Physical Description: Yellow cryst. (H<sub>2</sub>O)

Melting Point: Mp 176°

Hazard & Toxicity: LD<sub>50</sub> (rat, orl) 1394 mg/kg

Rare Chemicals Library: S62076-9

Supelco: R47-4205

>>Derivative: *N*-Ac

CAS Registry Number: 3484-26-2

Molecular Formula: C<sub>9</sub>H<sub>9</sub>N<sub>3</sub>O<sub>5</sub>

Molecular Weight: 239.187

Accurate Mass: 239.054222

Percentage Composition: C 45.19%; H 3.79%; N 17.57%; O 33.45%

Melting Point: Mp 159-160°

>>Derivative: *N*-Benzoyl

Molecular Formula: C<sub>14</sub>H<sub>11</sub>N<sub>3</sub>O<sub>5</sub>

Molecular Weight: 301.258

Accurate Mass: 301.069872

Percentage Composition: C 55.82%; H 3.68%; N 13.95%; O 26.55%

Melting Point: Mp 216-217°

References:

Channon, H.J. *et al.*, *Biochem. J.*, 1944, **38**, 70, (*synth, derivs*)

Noland, W.E. *et al.*, *J.O.C.*, 1965, **30**, 3457, (*derivs*)

Nielsen, A.T. *et al.*, *J.O.C.*, 1979, **44**, 2499, (*synth, pmr*)

Shevelev, S.A. *et al.*, *Synth. Commun.*, 2001, **31**, 2557-2561, (*synth, ir, pmr, cmr, ms*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, AJR750