



>>Entry Name: Acetoacetanilide

Synonym(s): 3-Oxo-*N*-phenylbutanamide, 9CI

CAS Registry Number: 102-01-2

PhNHCOCH₂COCH₃

Molecular Formula: C₁₀H₁₁NO₂

Molecular Weight: 177.202

Accurate Mass: 177.078979

Percentage Composition: C 67.78%; H 6.26%; N 7.90%; O 18.06%

Use/Importance: Coupling reagent for sulfa drugs (tlc sepn.)

Physical Description: Cryst. (petrol)

Melting Point: Mp 80° (86°)

Density: d²⁰ 1.26

Hazard & Toxicity: Fl. p. 185/163° (oc). Weak allergen. LD₅₀ (rat, orl) 5400 mg/kg

Aldrich: A873-2

Sigma: A1500

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1381A, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 363B, (ir)

Org. Synth., Coll. Vol., 3, 1955, 10, (synth, bibl)

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Hussein, S.M. *et al.*, *J. Het. Chem.*, 1988, **25**, 9, (rev)

Kubozono, Y. *et al.*, *Bull. Chem. Soc. Jpn.*, 1992, **65**, 3234, (cryst struct)

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