



>>Entry Name: 1,1,1-Trifluoro-3-phenyl-2-propanone

Synonym(s): Benzyl trifluoromethyl ketone

CAS Registry Number: 350-92-5

Related CAS Registry Numbers(s): 125774-47-2 125774-52-9

PhCH₂COCF₃

Molecular Formula: C₉H₇F₃O

Molecular Weight: 188.149

Accurate Mass: 188.044899

Percentage Composition: C 57.45%; H 3.75%; F 30.29%; O 8.50%

Physical Description: Liq.

Boiling Point: Bp₁₅ 72-75°

Refractive Index: n_D²⁵ 1.4432

Aldrich: 41678-9

>>Derivative: Oxime

Molecular Formula: C₉H₈F₃NO

Molecular Weight: 203.163

Accurate Mass: 203.055798

Percentage Composition: C 53.21%; H 3.97%; F 28.05%; N 6.89%; O 7.88%

Melting Point: Mp 40-42°

Boiling Point: Bp₃ 91-92°

>>Derivative: Semicarbazone

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 129-130°

References:

Nes, W.R. *et al.*, *J.A.C.S.*, 1950, **72**, 5409, (*synth, derivs*)

Begue, J.P. *et al.*, *J. Fluorine Chem.*, 1988, **39**, 271, (*synth*)

Quinze, K. *et al.*, *J. Fluorine Chem.*, 1989, **44**, 211, (*bibl, synth, ir, pmr, cmr*)

Grunewald, G.L. *et al.*, *J. Med. Chem.*, 1999, **42**, 3315-3323, (*synth, oxime, ir, pmr, cmr*)