



>>Entry Name: 4,4,4-Trifluoro-1-phenyl-1,3-butanedione, 9CI

Synonym(s): Benzoyltrifluoroacetone. 1-Phenyl-4,4,4-trifluoro-1,3-butanedione

CAS Registry Number: 326-06-7

PhCOCH₂COCF₃

Molecular Formula: C₁₀H₇F₃O₂

Molecular Weight: 216.159

Accurate Mass: 216.039814

Percentage Composition: C 55.57%; H 3.26%; F 26.37%; O 14.80%

Use/Importance: Used as a 0.03% soln. in butyl propionate for extraction-photometric detn. of U. Used to extract metals from waste, including plutonium and neptunium from nuclear waste. (Many patents inc. U.S. govt.)

Physical Description: Cryst.

Melting Point: Mp 38-40°

Boiling Point: Bp 224°

Solubility: Sol. EtOH, Me₂CO; insol. H₂O

Aldrich: 21704-2

Rare Chemicals Library: S28071-2

Sigma: B5875

>>Derivative: Oxime

Molecular Formula: C₁₀H₈F₃NO₂

Molecular Weight: 231.174

Accurate Mass: 231.050713

Percentage Composition: C 51.96%; H 3.49%; F 24.65%; N 6.06%; O 13.84%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 143.3-144.1°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 880B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 54C, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1264D, (*ir*)

Reid, J.C. *et al.*, *J.A.C.S.*, 1950, **72**, 2948, (*oxime*)

Shigematsu, T. *et al.*, *Bull. Chem. Soc. Jpn.*, 1964, **37**, 1333

Marsh, S.F. *et al.*, *Anal. Chim. Acta*, 1979, **105**, 439