



>>Entry Name: 1,1,1,5,5,5-Hexafluoro-2,4-pentanedione, 9CI

Synonym(s): Hexafluoroacetylacetone

CAS Registry Number: 1522-22-1

$\text{F}_3\text{CCOCH}_2\text{COCF}_3$

Molecular Formula:  $\text{C}_5\text{H}_2\text{F}_6\text{O}_2$

Molecular Weight: 208.06

Accurate Mass: 207.995898

Percentage Composition: C 28.86%; H 0.97%; F 54.79%; O 15.38%

Use/Importance: Used as 1% EtOH soln. for extraction separation of Fe(III), Be ( $\text{C}_6\text{H}_6$ ); fluorimetric detn. of Eu, Tb, Sm

Physical Description: Liq. with irritant odour

Melting Point: Mp 90 dec.° (as dihydrate)

Boiling Point: Bp 70-71° (63-65°)

pKa Value:  $\text{p}K_{\text{a}}$  4.42 (25°)

Aldrich: 23830-9

Fluka: 52503

Sigma: H4013

#### References:

*Aldrich Library of  $^{13}\text{C}$  and  $^1\text{H}$  FT NMR Spectra*, 1992, **1**, 662C, (nmr)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 426A, (ir)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 511D, (ir)

Henne, A. *et al.*, *J.A.C.S.*, 1947, **69**, 1819; 1956, **78**, 2790, (synth)

Scribner, W.G. *et al.*, *Anal. Chem.*, 1965, **37**, 1136; 1966, **38**, 1779, (detn, Be)

Williams, D.E. *et al.*, *Anal. Chem.*, 1971, **43**, 139, (detn, Eu, Tb)

Williams, D.E. *et al.*, *Mikrochim. Acta*, 1972, 194, (detn, Sm)

Turoff, M.L. *et al.*, *Talanta*, 1977, **24**, 567, (detn, Fe)

Lo, J.G. *et al.*, *J. Chromatogr. Sci.*, 1980, **18**, 359, (use)