



>>Entry Name: 2-Methyl-3-oxo-4,4,4-trifluorobutanoic acid

Synonym(s): α -Methyl-4,4,4-trifluoroacetoacetic acid. 2-(Trifluoroacetyl)propanoic acid

Related CAS Registry Numbers(s): 75631-72-0

$\text{F}_3\text{CCOCH}(\text{CH}_3)\text{COOH}$

Molecular Formula: $\text{C}_5\text{H}_5\text{F}_3\text{O}_3$

Molecular Weight: 170.088

Accurate Mass: 170.019079

Percentage Composition: C 35.31%; H 2.96%; F 33.51%; O 28.22%

>>Derivative: Et ester

CAS Registry Number: 344-00-3

Molecular Formula: $\text{C}_7\text{H}_9\text{F}_3\text{O}_3$

Molecular Weight: 198.141

Accurate Mass: 198.050379

Percentage Composition: C 42.43%; H 4.58%; F 28.76%; O 24.22%

Boiling Point: Bp 144-146°. Bp₂₆ 57.8°

Refractive Index: n_D^{20} 1.3650

Other: Oakwood 1554

>>Derivative: Et ester, Cu(II) chelate

Melting Point: Mp 131°

>>Derivative: Et ester, 2,4-dinitrophenylhydrazone

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 70.5-71.5°

References:

McBee, E.T. *et al.*, *J.A.C.S.*, 1956, **78**, 4053

Burdon, J. *et al.*, *Tetrahedron*, 1964, **20**, 2163

Aubert, C. *et al.*, *J. Fluorine Chem.*, 1989, **44**, 361, (*synth, cmr, F-19 nmr*)