



>>Entry Name: 4,4,4-Trifluoro-3-oxobutanoic acid, 9CI

Synonym(s): Trifluoroacetoacetic acid

CAS Registry Number: 400-36-2

Related CAS Registry Numbers(s): 2249-25-4 26736-15-2 65145-41-7 83097-87-4 89129-76-0 92980-11-5 108550-89-6 118993-06-9

F3CCOCH2COOH

Molecular Formula: C4H3F3O3

Molecular Weight: 156.061

Accurate Mass: 156.003429

Percentage Composition: C 30.79%; H 1.94%; F 36.52%; O 30.76%

>>Derivative: Me ester

CAS Registry Number: 83643-84-9

Molecular Formula: C5H5F3O3

Molecular Weight: 170.088

Accurate Mass: 170.019079

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

Boiling Point: Bp₇₄₅ 116°

>>Derivative: Et ester

CAS Registry Number: 372-31-6

Molecular Formula: C6H7F3O3

Molecular Weight: 184.115

Accurate Mass: 184.034729

Percentage Composition: C 39.14%; H 3.83%; F 30.96%; O 26.07%

Boiling Point: Bp 132°

Refractive Index: n_D²⁵ 1.3740

Hazard & Toxicity: A method reported by McBee *et al* (1953) is reported to cause explosions

Aldrich: E5020-5

Fluka: 91670

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

Physical Description: Pale yellow needles (EtOH)

Melting Point: Mp 103.5-105°

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 26717-75-9

Molecular Formula: C8H11F3O3

Molecular Weight: 212.168

Accurate Mass: 212.066029

Percentage Composition: C 45.29%; H 5.23%; F 26.86%; O 22.62%

Melting Point: Mp 69.5-70° (hydrate)

>>Derivative: Di-Et acetal, Et ester

Synonym(s): Ethyl 3,3-diethoxy-4,4,4-trifluorobutanoate

Molecular Formula: C10H17F3O4

Molecular Weight: 258.237

Accurate Mass: 258.107894

Percentage Composition: C 46.51%; H 6.64%; F 22.07%; O 24.78%

Boiling Point: Bp₈ 72-76°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1099C, (*nmr*, *Et ester*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 744A, (*ir*, *Et ester*)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 402F, (*ir*, *Et ester*)

Burdon, J. *et al.*, *Tetrahedron*, 1964, **20**, 2163, (*Et ester*, *synth*)

Grell, W. *et al.*, *Annalen*, 1966, **693**, 134, (*di-Et acetal Et ester*)

Slusarczuk, G.M.J. *et al.*, *J.O.C.*, 1971, **36**, 37, (*Et ester*, *tert-butyl ester*, *synth*)

Saloutin, V.I. *et al.*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1984, 1106; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1984, 1016, (*Me ester*, *synth*)

Geraldes, C.F.G.C. *et al.*, *J. Mol. Struct.*, 1990, **238**, 335, (*tautom*, *cmr*, *Et ester*)

Commercially available and/or commonly cited compound for which no useful literature data is available, 1995, (*di-Me acetal Et ester*)