



>>Entry Name: 3,3,3-Trifluoro-2-oxopropanoic acid, 9CI

Synonym(s): Trifluoropyruvic acid

CAS Registry Number: 431-72-1

F₃CCOCOOH

Molecular Formula: C₃HF₃O₃

Molecular Weight: 142.034

Accurate Mass: 141.987779

Percentage Composition: C 25.37%; H 0.71%; F 40.13%; O 33.79%

>>Derivative: Covalent hydrate

Synonym(s): 3,3,3-Trifluoro-2,2-dihydroxypropanoic acid

CAS Registry Number: 10321-14-9

Molecular Formula: C₃H₃F₃O₄

Molecular Weight: 160.05

Accurate Mass: 159.998344

Percentage Composition: C 22.51%; H 1.89%; F 35.61%; O 39.99%

Physical Description: Hygroscopic cryst. (EtOAc/CHCl₃)

Melting Point: Mp 124-126° (119.5-122.5°)

Rare Chemicals Library: S13901-7

>>Derivative: Semicarbazone

Physical Description: Cryst. (H₂O)

Melting Point: Mp 217-219°

>>Derivative: Me ester

CAS Registry Number: 13089-11-7

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%

Physical Description: Liq.

Boiling Point: Bp 85-87°

Refractive Index: n_D²⁰ 1.3280

>>Derivative: Et ester

CAS Registry Number: 13081-18-0

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%

Physical Description: Liq.

Boiling Point: Bp 95-98°

Refractive Index: n_D²⁰ 1.3350

Other: Oakwood: 3224

>>Derivative: Fluoride

CAS Registry Number: 7309-82-2

Molecular Formula: C₃F₄O₂

Molecular Weight: 144.025

Accurate Mass: 143.983442

Percentage Composition: C 25.02%; F 52.76%; O 22.22%

Physical Description: Liq. or gas

Boiling Point: Bp 9-10°