



>>Entry Name: 3,3,3-Trifluoropropanoic acid

Synonym(s): β,β,β -Trifluoropropionic acid

CAS Registry Number: 2516-99-6

$\text{F}_3\text{CCH}_2\text{COOH}$

Molecular Formula: $\text{C}_3\text{H}_3\text{F}_3\text{O}_2$

Molecular Weight: 128.051

Accurate Mass: 128.008514

Percentage Composition: C 28.14%; H 2.36%; F 44.51%; O 24.99%

Melting Point: Mp 9.7°

Boiling Point: Bp₇₄₆ 144.8°

>>Derivative: NH_4 salt

Boiling Point: Bp₂₁ 136° subl.

>>Derivative: Aniline salt

Physical Description: Cryst. (EtOH)

Melting Point: Mp 116°

>>Derivative: S-Benzylthiouronium salt

Physical Description: Cryst. (EtOH)

Melting Point: Mp 176°

>>Derivative: Me ester

CAS Registry Number: 18830-44-9

Molecular Formula: $\text{C}_4\text{H}_5\text{F}_3\text{O}_2$

Molecular Weight: 142.077

Accurate Mass: 142.024164

Percentage Composition: C 33.82%; H 3.55%; F 40.12%; O 22.52%

Boiling Point: Bp 95-96°

>>Derivative: Et ester

CAS Registry Number: 352-23-8

Molecular Formula: $\text{C}_5\text{H}_7\text{F}_3\text{O}_2$

Molecular Weight: 156.104

Accurate Mass: 156.039814

Percentage Composition: C 38.47%; H 4.52%; F 36.51%; O 20.50%

Boiling Point: Bp 97-98°. Bp₁₂ 50°

>>Derivative: Fluoride

CAS Registry Number: 85345-75-1

Molecular Formula: $\text{C}_3\text{H}_2\text{F}_4\text{O}$

Molecular Weight: 130.042

Accurate Mass: 130.004177

Percentage Composition: C 27.71%; H 1.55%; F 58.44%; O 12.30%

Physical Description: Liq.

>>Derivative: Chloride

Molecular Formula: $\text{C}_3\text{H}_2\text{ClF}_3\text{O}$

Molecular Weight: 146.496

Accurate Mass: 145.974626

Percentage Composition: C 24.60%; H 1.38%; Cl 24.20%; F 38.91%; O 10.92%

Boiling Point: Bp₇₄₅ 70.3°