



>>Entry Name: 4,4,4-Trifluoro-2-butenic acid

CAS Registry Number: 71027-02-6

$\text{F}_3\text{CCH}=\text{CHCOOH}$

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

Molecular Weight: 140.062

Accurate Mass: 140.008514

Percentage Composition: C 34.30%; H 2.16%; F 40.69%; O 22.85%

>>Variant: (*E*)-form

Synonym(s): 4,4,4-Trifluorocrotonic acid

CAS Registry Number: 406-94-0

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

Molecular Weight: 140.062

Accurate Mass: 140.008514

Percentage Composition: C 34.30%; H 2.16%; F 40.69%; O 22.85%

Physical Description: Cryst. (petrol)

Melting Point: Mp 55-56°

Boiling Point: Bp 145-150° (68.0-69.0°)

>>Derivative: Et ester

CAS Registry Number: 25597-16-4

Molecular Formula: $\text{C}_6\text{H}_7\text{F}_3\text{O}_2$

Molecular Weight: 168.115

Accurate Mass: 168.039814

Percentage Composition: C 42.87%; H 4.20%; F 33.90%; O 19.03%

Physical Description: Liq.

Boiling Point: Bp 112.5°

Density: d_4^{25} 1.13

Aldrich: 26969-7

>>Derivative: Amide

CAS Registry Number: 590-76-1

Molecular Formula: $\text{C}_4\text{H}_4\text{F}_3\text{NO}$

Molecular Weight: 139.077

Accurate Mass: 139.024498

Percentage Composition: C 34.54%; H 2.90%; F 40.98%; N 10.07%; O 11.50%

Physical Description: Cryst. (Et_2O /petrol)

Melting Point: Mp 146.5-147.5°

Other: Oakwood 1564

>>Derivative: Nitrile

Synonym(s): 1-Cyano-2-(trifluoromethyl)ethylene

CAS Registry Number: 406-86-0

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

Molecular Weight: 121.062

Accurate Mass: 121.013933

Percentage Composition: C 39.69%; H 1.67%; F 47.08%; N 11.57%

Physical Description: Liq.

Boiling Point: Bp 84-85°. Bp 110-120°

Other: Oakwood 1563

>>Variant: (*Z*)-form

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

Molecular Weight: 140.062

Accurate Mass: 140.008514

Percentage Composition: C 34.30%; H 2.16%; F 40.69%; O 22.85%

Physical Description: Liq.

Boiling Point: Bp₁₁ 66-69°