



>> / Name: **3-Amino-4,4,4-trifluoro-2-butenic acid**, 9CI

Synonym(s): 3-Amino-4,4,4-trifluorocrotonic acid, 8CI

**CAS Registry Number:** 158756-18-4

F3CC(NH2)=CHCOOH

**Molecular Formula:** C<sub>4</sub>H<sub>4</sub>F<sub>3</sub>NO<sub>2</sub>

**Molecular Weight:** 155.076

**Accurate Mass:** 155.019413

**Percentage Composition:** C 30.98%; H 2.60%; F 36.75%; N 9.03%; O 20.63%

>>Derivative: Me ester

**CAS Registry Number:** 107638-19-7

**Molecular Formula:** C<sub>5</sub>H<sub>6</sub>F<sub>3</sub>NO<sub>2</sub>

**Molecular Weight:** 169.103

**Accurate Mass:** 169.035063

**Percentage Composition:** C 35.51%; H 3.58%; F 33.70%; N 8.28%; O 18.92%

**Physical Description:** Cryst. (hexane)

**Melting Point:** Mp 50-52°

>>Derivative: Et ester

**CAS Registry Number:** 372-29-2

**Molecular Formula:** C<sub>6</sub>H<sub>8</sub>F<sub>3</sub>NO<sub>2</sub>

**Molecular Weight:** 183.13

**Accurate Mass:** 183.050713

**Percentage Composition:** C 39.35%; H 4.40%; F 31.12%; N 7.65%; O 17.47%

**Boiling Point:** Bp<sub>15</sub> 83°

**Refractive Index:** n<sub>D</sub><sup>20</sup> 1.4420

**Aldrich:** 44369-7

>>Derivative: Amide

**CAS Registry Number:** 107638-26-6

**Molecular Formula:** C<sub>4</sub>H<sub>5</sub>F<sub>3</sub>N<sub>2</sub>O

**Molecular Weight:** 154.091

**Accurate Mass:** 154.035397

**Percentage Composition:** C 31.18%; H 3.27%; F 36.99%; N 18.18%; O 10.38%

**Physical Description:** Cryst. (hexane)

**Melting Point:** Mp 69-71°

#### References:

Lutz, A. *et al.*, *J. Het. Chem.*, 1972, **9**, 513, (*Et ester*)

Pashkevich, K.I. *et al.*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1986, **35**, 1586; *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1986, **35**, 1438, (*derivs*)