



>>Entry 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

$\text{F}_3\text{CC}(\text{NH}_2)=\text{CHCOOH}$

Molecular Formula: $\text{C}_4\text{H}_4\text{F}_3\text{NO}_2$

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: $\text{C}_5\text{H}_6\text{F}_3\text{NO}_2$

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: $\text{C}_6\text{H}_8\text{F}_3\text{NO}_2$

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: Bp₁₅ 83°

Refractive Index: n_D²⁰ 1.4420

Aldrich: 44369-7

>>Derivative: Amide

CAS Registry Number: 107638-26-6

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

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*)