



>>Entry Name: 4,4,4-Trifluorobutanoic acid

CAS Registry Number: 406-93-9

F3CCH2CH2COOH

Molecular Formula: C4H5F3O2

Molecular Weight: 142.077

Accurate Mass: 142.024164

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

Melting Point: Mp 33.2°

Boiling Point: Bp₁₈ 78°. Bp 166.6°

Rare Chemicals Library: S81893-3

>>Derivative: Et ester

CAS Registry Number: 371-26-6

Molecular Formula: C6H9F3O2

Molecular Weight: 170.131

Accurate Mass: 170.055464

Percentage Composition: C 42.36%; H 5.33%; F 33.50%; O 18.81%

Boiling Point: Bp 127°

Aldrich: 44370-0

Rare Chemicals Library: S60017-2

Other: Oakwood 1498

>>Derivative: Chloride

Molecular Formula: C4H4ClF3O

Molecular Weight: 160.523

Accurate Mass: 159.990276

Percentage Composition: C 29.93%; H 2.51%; Cl 22.09%; F 35.51%; O 9.97%

Boiling Point: Bp₇₄₅ 103°

>>Derivative: Amide

Molecular Formula: C4H6F3NO

Molecular Weight: 141.093

Accurate Mass: 141.040148

Percentage Composition: C 34.05%; H 4.29%; F 40.40%; N 9.93%; O 11.34%

Physical Description: Cryst.

Melting Point: Mp 136.4°

References:

McBee, E.T. *et al.*, *J.A.C.S.*, 1948, **70**, 2910; 1954, **76**, 3722, (*synth*)

Henne, A.L. *et al.*, *J.A.C.S.*, 1951, **73**, 2323; 1955, **77**, 1901, (*derivs, props*)

Fuchikami, T. *et al.*, *J.O.C.*, 1983, **48**, 3803, (*ester, pmr, F-19 nmr, ir, ms*)

Jacobs, R.T. *et al.*, *J. Med. Chem.*, 1994, **37**, 1282, (*synth, pmr*)