



>>Entry Name: 3-(Trifluoromethyl)benzoic acid, 9CI

Synonym(s): α,α,α -Trifluoro-*m*-toluic acid, 8CI. Benzotrifluoride-3-carboxylic acid

CAS Registry Number: 454-92-2

Molecular Formula: $C_8H_5F_3O_2$

Molecular Weight: 190.121

Accurate Mass: 190.024164

Percentage Composition: C 50.54%; H 2.65%; F 29.98%; O 16.83%

Use/Importance: Reference material used in elemental microanalysis

Physical Description: Cryst. (CCl_4)

Melting Point: Mp 104°

Aldrich: 18834-4

Fluka: 91770

Sigma: C7875

>>Derivative: Me ester

CAS Registry Number: 2557-13-3

Molecular Formula: $C_9H_7F_3O_2$

Molecular Weight: 204.148

Accurate Mass: 204.039814

Percentage Composition: C 52.95%; H 3.46%; F 27.92%; O 15.67%

Boiling Point: Bp₂₀ 93-95°

Aldrich: 40043-2

Fluka: 91785

>>Derivative: Et ester

CAS Registry Number: 76783-59-0

Molecular Formula: $C_{10}H_9F_3O_2$

Molecular Weight: 218.175

Accurate Mass: 218.055464

Percentage Composition: C 55.05%; H 4.16%; F 26.12%; O 14.67%

Boiling Point: Bp₁₀ 100-101°

>>Derivative: Chloride

CAS Registry Number: 2251-65-2

Molecular Formula: $C_8H_4ClF_3O$

Molecular Weight: 208.567

Accurate Mass: 207.990276

Percentage Composition: C 46.07%; H 1.93%; Cl 17.00%; F 27.33%; O 7.67%

Physical Description: Oil

Boiling Point: Bp₁₆ 79-80°

Aldrich: 25027-9

Fluka: 91830

Sigma: T2002

>>Derivative: Nitrile

Synonym(s): 1-Cyano-3-(trifluoromethyl)benzene

CAS Registry Number: 368-77-4

Molecular Formula: $C_8H_4F_3N$

Molecular Weight: 171.121

Accurate Mass: 171.029583

Percentage Composition: C 56.15%; H 2.36%; F 33.31%; N 8.19%

Boiling Point: Bp₄₀ 94-95°

Aldrich: 17290-1

Fluka: 91800

Sigma: T1752

References: