



>>Entry Name: 4-(Trifluoromethyl)benzoic acid, 9Cl

Synonym(s): α,α,α -Trifluoro-*p*-toluic acid, 8Cl. Benzotrifluoride-4-carboxylic acid

CAS Registry Number: 455-24-3

Molecular Formula: C₈H₅F₃O₂

Molecular Weight: 190.121

Accurate Mass: 190.024164

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

Physical Description: Cryst.

Melting Point: Mp 220-221°

Aldrich: 19689-4

Fluka: 91780

>>Derivative: Me ester

CAS Registry Number: 2967-66-0

Molecular Formula: C₉H₇F₃O₂

Molecular Weight: 204.148

Accurate Mass: 204.039814

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

Melting Point: Mp 13-14°

Boiling Point: Bp₂₁ 94-95°

Refractive Index: n_D²⁰ 1.4510

Aldrich: 33344-1

>>Derivative: Et ester

CAS Registry Number: 583-02-8

Molecular Formula: C₁₀H₉F₃O₂

Molecular Weight: 218.175

Accurate Mass: 218.055464

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

Boiling Point: Bp₁₂ 90-94°

>>Derivative: Chloride

CAS Registry Number: 329-15-7

Molecular Formula: C₈H₄ClF₃O

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%

Use/Importance: Used to derivatise amines for gc analysis

Physical Description: Liq.

Boiling Point: Bp₁₆ 78-79°. Bp₁₂ 74-75°

Density: d₄²⁵ 1.4035

Refractive Index: n_D²⁰ 1.4755

Aldrich: 24947-5

Fluka: 91840

Sigma: T7760

>>Derivative: Amide

CAS Registry Number: 1891-90-3

Molecular Formula: C₈H₆F₃NO

Molecular Weight: 189.137

Accurate Mass: 189.040148

Percentage Composition: C 50.80%; H 3.20%; F 30.13%; N 7.41%; O 8.46%

Melting Point: Mp 184-186°

Aldrich: 28235-9

Sigma: T6027