



>>Entry Name: 2,4,5-Trifluorobenzoic acid

CAS Registry Number: 446-17-3

Molecular Formula: $C_7H_3F_3O_2$

Molecular Weight: 176.095

Accurate Mass: 176.008514

Percentage Composition: C 47.75%; H 1.72%; F 32.37%; O 18.17%

Physical Description: Cryst.

Melting Point: Mp 97-98°

Aldrich: 32815-4

Fluka: 91697

>>Derivative: Me ester

CAS Registry Number: 20372-66-1

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%

Physical Description: Liq.

Boiling Point: Bp₁₀₀ 130-135°

>>Derivative: Amide

CAS Registry Number: 98349-23-6

Molecular Formula: $C_7H_4F_3NO$

Molecular Weight: 175.11

Accurate Mass: 175.024498

Percentage Composition: C 48.01%; H 2.30%; F 32.55%; N 8.00%; O 9.14%

Physical Description: No phys. props. accessible

>>Derivative: Nitrile

Synonym(s): 2,4,5-Trifluorobenzonitrile. 1-Cyano-2,4,5-trifluorobenzene

CAS Registry Number: 98349-22-5

Molecular Formula: $C_7H_2F_3N$

Molecular Weight: 157.095

Accurate Mass: 157.013933

Percentage Composition: C 53.52%; H 1.28%; F 36.28%; N 8.92%

Physical Description: Liq.

Aldrich: 32820-0

References:

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De Graw, J.I. *et al.*, *J. Chem. Eng. Data*, 1968, **13**, 587, (*synth, deriv, pmr*)
Sanchez, J.P. *et al.*, *J. Med. Chem.*, 1988, **31**, 983, (*synth, deriv, pmr*)
Chu, D.T.W. *et al.*, *J. Med. Chem.*, 1991, **34**, 168, (*synth, pmr*)
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