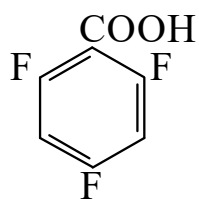




>>Entry Name: 2,4,6-Trifluorobenzoic acid



CAS Registry Number: 28314-80-9

Related CAS Registry Numbers(s): 79538-28-6

Molecular Formula: C₇H₃F₃O₂

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. (H₂O)

Melting Point: Mp 143-145°

Aldrich: 34578-4

>>Derivative: Chloride

CAS Registry Number: 79538-29-7

Molecular Formula: C₇H₂ClF₃O

Molecular Weight: 194.54

Accurate Mass: 193.974626

Percentage Composition: C 43.22%; H 1.04%; Cl 18.22%; F 29.30%; O 8.22%

Physical Description: Liq.

>>Derivative: Nitrile

Synonym(s): 2-Cyano-1,3,5-trifluorobenzene

CAS Registry Number: 96606-37-0

Molecular Formula: C₇H₂F₃N

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.

Boiling Point: Bp 92°

References:

Sugawara, S. *et al.*, *CA*, 1970, **73**, 77636b, (*synth*)

Eur. Pat., 1982, 60 617; *CA*, **98**, 125610d, (*synth, derivs*)

Japan. Pat., 1985, 85 23 358; *CA*, **102**, 220595n, (*synth, derivs*)