



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

Synonym(s): α,α,α -Trifluoro-*m*-cresol, 8CI. *m*-Hydroxybenzotrifluoride

CAS Registry Number: 98-17-9

Molecular Formula: $C_7H_5F_3O$

Molecular Weight: 162.111

Accurate Mass: 162.029249

Percentage Composition: C 51.86%; H 3.11%; F 35.16%; O 9.87%

Melting Point: Mp -1.8°

Boiling Point: Bp 178-179°

Hazard & Toxicity: Irritant

Aldrich: 15603-5

Fluka: 54820

Sigma: H5751

>>Derivative: Me ether

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

CAS Registry Number: 454-90-0

Molecular Formula: $C_8H_7F_3O$

Molecular Weight: 176.138

Accurate Mass: 176.044899

Percentage Composition: C 54.55%; H 4.01%; F 32.36%; O 9.08%

Physical Description: Liq.

Aldrich: 21310-1

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 249A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1074C, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1006C, (*ir*)

Swarts, F., *Bull. Acad. R. Med. Belg.*, 1913, 241; *Chem.-Ztg.*, 1913, 760, (*synth*)

Swarts, F., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1913, **32**, 71, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, TKE750