



Aldrich: 12084-7

Fluka: 46740

Sigma: F0251

>> **Derivative:** Amide

CAS Registry Number: 445-28-3

Molecular Formula: C₇H₆FNO

Molecular Weight: 139.129

Accurate Mass: 139.043342

Percentage Composition: C 60.43%; H 4.35%; F 13.66%; N 10.07%; O 11.50%

Melting Point: Mp 116°. Mp 117-119°

Aldrich: 12170-3

>> **Derivative:** Nitrile

Synonym(s): 2-Fluorobenzonitrile. 1-Cyano-2-fluorobenzene

CAS Registry Number: 394-47-8

Molecular Formula: C₇H₄FN

Molecular Weight: 121.114

Accurate Mass: 121.032777

Percentage Composition: C 69.42%; H 3.33%; F 15.69%; N 11.56%

Boiling Point: Bp₂₁ 90°

Aldrich: 19664-9

Fluka: 46675

>> **Derivative:** Anhydride

CAS Registry Number: 64508-63-0

Molecular Formula: C₁₄H₈F₂O₃

Molecular Weight: 262.212

Accurate Mass: 262.044151

Percentage Composition: C 64.13%; H 3.08%; F 14.49%; O 18.31%

Physical Description: Cryst. (C₆H₆/hexane)

Melting Point: Mp 58-59°

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 186D; 341A; 367C; 443B; 1509C
- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 443B; 1064A; 1338A; 1387C; 1509C; **3**, 1407A, (*nmr, derivs*)
- Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 1390D; 1407A, (*ir*)
- Dippy, J. *et al.*, *J.C.S.*, 1934, 1466
- Borsche, W. *et al.*, *Annalen*, 1941, **546**, 273, (*nitrile*)
- Tomasik, P. *et al.*, *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, 1974, **22**, 1065, (*uv*)
- Ferguson, G. *et al.*, *Cryst. Struct. Commun.*, 1975, **4**, 389, (*cryst struct*)
- Sterk, H. *et al.*, *Org. Magn. Reson.*, 1975, **7**, 274, (*nmr*)
- Cohen, T. *et al.*, *J.O.C.*, 1978, **43**, 837, (*anhydride*)
- Ichikawa, H. *et al.*, *Org. Mass Spectrom.*, 1978, **13**, 389, (*ms*)
- Zweig, A. *et al.*, *J.O.C.*, 1980, **45**, 3597, (*synth*)
- Kato, Y. *et al.*, *Bull. Chem. Soc. Jpn.*, 1982, **55**, 1643
- Berkovitch-Yellin, Z. *et al.*, *J.A.C.S.*, 1982, **104**, 4052, (*cryst struct*)
- Noto, R. *et al.*, *J.C.S. Perkin 2*, 1988, 887, (*cmr*)
- Fifolt, M.J. *et al.*, *J.O.C.*, 1989, **54**, 3019, (*F-19 nmr*)
- McKillop, A. *et al.*, *Tetrahedron*, 1989, **45**, 3299, (*synth*)
- Schlosser, M. *et al.*, *Synlett*, 1990, 747, (*synth*)
- Milner, D.J., *Synth. Commun.*, 1992, **22**, 73, (*synth*)
- Shibakami, M. *et al.*, *Acta Cryst. C*, 1995, **51**, 326, (*cryst struct, Ph ester*)
- Abraham, R.J. *et al.*, *J.C.S. Perkin 2*, 1997, 41-49, (*Me ester, pmr, cmr, F-19 nmr*)
- Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, FGH000; FGP000