



>>Entry Name: 3-Fluoro-1,2-benzenedicarboxylic acid, 9CI

Synonym(s): 3-Fluorophthalic acid, 8CI

CAS Registry Number: 1583-67-1

Structure by analogy with 2-Fluoro-1,3-benzenedicarboxylic acid, [DZL42-O](#)

Molecular Formula: C₈H₅FO₄

Molecular Weight: 184.123

Accurate Mass: 184.017188

Percentage Composition: C 52.19%; H 2.74%; F 10.32%; O 34.76%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 167-168°

Aldrich: 33471-5

>>Derivative: Anhydride

CAS Registry Number: 652-39-1

Molecular Formula: C₈H₃FO₃

Molecular Weight: 166.108

Accurate Mass: 166.006623

Percentage Composition: C 57.85%; H 1.82%; F 11.44%; O 28.90%

Physical Description: Cryst. (toluene or Ac₂O)

Melting Point: Mp 160°

Boiling Point: Bp₇₃₀ 281-283°

Aldrich: 46770-7

>>Derivative: Dinitrile

Synonym(s): 1,2-Dicyano-3-fluorobenzene

CAS Registry Number: 65610-13-1

Molecular Formula: C₈H₃FN₂

Molecular Weight: 146.123

Accurate Mass: 146.028026

Percentage Composition: C 65.76%; H 2.07%; F 13.00%; N 19.17%

Physical Description: Cryst. (hexane)

Melting Point: Mp 61°

References:

Heller, A., *J.O.C.*, 1960, **25**, 834, (*synth*)

Newman, M.S. *et al.*, *J.O.C.*, 1961, **26**, 3210, (*synth*)

Valkanas, G. *et al.*, *J.C.S.*, 1963, 3475, (*synth*)

Oksengendler, I.G. *et al.*, *J. Org. Chem. USSR (Engl. Transl.)*, 1977, **13**, 2085, (*deriv*)

Soucy, C. *et al.*, *J.O.C.*, 1987, **52**, 129, (*deriv, synth, pmr, cmr, ir, ms*)