



>>Entry Name: **2-Amino-4-(trifluoromethyl)benzoic acid**, 9CI

Synonym(s): 2-Amino- α,α,α -trifluoro-*p*-toluic acid, 8CI. 4-(Trifluoromethyl)anthranilic acid

CAS Registry Number: 402-13-1

Molecular Formula: $C_8H_6F_3NO_2$

Molecular Weight: 205.136

Accurate Mass: 205.035063

Percentage Composition: C 46.84%; H 2.95%; F 27.78%; N 6.83%; O 15.60%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 175-177°

>>Derivative: Me ester

CAS Registry Number: 61500-87-6

Molecular Formula: $C_9H_8F_3NO_2$

Molecular Weight: 219.163

Accurate Mass: 219.050713

Percentage Composition: C 49.32%; H 3.68%; F 26.01%; N 6.39%; O 14.60%

Physical Description: Cryst. (hexane)

Melting Point: Mp 60-62°

References:

Hauptschein, M. *et al.*, *J.A.C.S.*, 1954, **76**, 1051, (*synth*)

Simet, L., *J.O.C.*, 1963, **28**, 3580, (*synth*)

Hill, D.T. *et al.*, *J. Med. Chem.*, 1983, **26**, 865, (*ester*)

Barlin, G.B. *et al.*, *Aust. J. Chem.*, 1990, **43**, 311, (*synth, ir, pmr*)

Norman, M.H. *et al.*, *J. Med. Chem.*, 1996, **39**, 1172, (*synth*)