



>>Entry Name: 4-Nitro-3-(trifluoromethyl)aniline

Synonym(s): 4-Nitro-3-(trifluoromethyl)benzenamine, 9CI. α,α,α -Trifluoro-4-nitro-*m*-toluidine, 8CI. 5-Amino-2-nitrobenzotrifluoride

CAS Registry Number: 393-11-3

Related CAS Registry Numbers(s): 17227-42-8 35844-18-9

Molecular Formula: $C_7H_5F_3N_2O_2$

Molecular Weight: 206.124

Accurate Mass: 206.030312

Percentage Composition: C 40.79%; H 2.44%; F 27.65%; N 13.59%; O 15.52%

Use/Importance: Flutamide metabolite in plasma and urine

Physical Description: Brilliant yellow needles (EtOH aq. or H_2O)

Melting Point: Mp 129° (124-126°)

pKa Value: $pK_a -0.05$

Aldrich: A6880-7

Fluka: 8875

Rare Chemicals Library: S41398-4

>>Derivative: *N*-Ac

CAS Registry Number: 393-12-4

Molecular Formula: $C_9H_7F_3N_2O_3$

Molecular Weight: 248.161

Accurate Mass: 248.040877

Percentage Composition: C 43.56%; H 2.84%; F 22.97%; N 11.29%; O 19.34%

Physical Description: Yellow cryst.

Melting Point: Mp 108-109°

References:

Pouterman, E. *et al.*, *Helv. Chim. Acta*, 1947, **30**, 107, (*synth*)

Jones, R.G., *J.A.C.S.*, 1947, **69**, 2346, (*synth*)

Maginnity, P.M. *et al.*, *J.A.C.S.*, 1951, **73**, 3579, (*synth*)

Caldwell, W.T. *et al.*, *J.A.C.S.*, 1951, **73**, 5125, (*synth*)

Smith, F. *et al.*, *J.C.S.*, 1951, 1701, (*uv*)

Randle, R.R. *et al.*, *J.C.S.*, 1952, 4153; 1955, 1311, (*ir*)

Forbes, E.J. *et al.*, *Tetrahedron*, 1960, **8**, 67, (*synth*)

Idoux, J.P. *et al.*, *J.O.C.*, 1968, **33**, 3498, (*synth*, *uv*)