



>>Entry Name: 2-Nitro-4-(trifluoromethyl)aniline

Synonym(s): 2-Nitro-4-(trifluoromethyl)benzenamine, 9CI. α,α,α -Trifluoro-2-nitro-*p*-toluidine, 8CI

CAS Registry Number: 400-98-6

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%

Physical Description: Yellow cryst. (EtOH aq.)

Melting Point: Mp 108-109°

pKa Value: $pK_a -2.61$ (25°, HClO₄)

Aldrich: A6860-2

Fluka: 8870

Sigma: A1525

>>Derivative: *N*-Ac

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: Solid

Melting Point: Mp 113°

>>Derivative: *N*-Trifluoroacetyl

Molecular Formula: $C_9H_4F_6N_2O_3$

Molecular Weight: 302.133

Accurate Mass: 302.012611

Percentage Composition: C 35.78%; H 1.33%; F 37.73%; N 9.27%; O 15.89%

Physical Description: Solid

Melting Point: Mp 65-66°

References:

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Hambly, A.N. *et al.*, *Aust. J. Chem.*, 1964, **17**, 860, (*ir*)

Schneck, J.O. *et al.*, *J.O.C.*, 1965, **30**, 3504, (*synth*, *uv*, *ir*)

Filleux-Blanchard, M.L. *et al.*, *Org. Magn. Reson.*, 1973, **5**, 221, (*pmr*)

Schuster, I.I.M., *J. Magn. Reson.*, 1975, **17**, 104, (*cmr*, *F-19 nmr*)

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