



>>Entry Name: 1-Chloro-4-nitro-2-(trifluoromethyl)benzene

Synonym(s): 2-Chloro- α,α,α -trifluoro-5-nitrotoluene, 8Cl. 2-Chloro-5-nitrobenzotrifluoride

CAS Registry Number: 777-37-7

Structure by analogy with 1-Chloro-2-nitro-4-(trifluoromethyl)benzene, [DSX66-J](#)

Molecular Formula: $C_7H_3ClF_3NO_2$

Molecular Weight: 225.554

Accurate Mass: 224.98044

Percentage Composition: C 37.28%; H 1.34%; Cl 15.72%; F 25.27%; N 6.21%; O 14.19%

Melting Point: Fp -21.7° . Mp $21.5-22.5^\circ$

Boiling Point: Bp 231.9° . Bp₈ 100° . Bp_{2.5} $64-66^\circ$ (lit. gives a pressure range)

Density: d_4^{30} 1.504

Hazard & Toxicity: Fl. p. 135°

Aldrich: C6040-6

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 721C, (*nmr*)

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Stacy, G. *et al.*, *J.O.C.*, 1957, **22**, 298, (*synth*)

Filler, R. *et al.*, *J.O.C.*, 1961, **26**, 2707, (*synth*)

Castellano, S.M. *et al.*, *Can. J. Chem.*, 1969, **47**, 3313, (*pmr*)

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