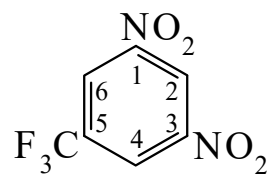




>>Entry Name: **1,3-Dinitro-5-(trifluoromethyl)benzene**

Synonym(s): α,α,α -Trifluoro-3,5-dinitrotoluene. 3,5-Dinitrobenzotrifluoride



CAS Registry Number: 401-99-0

Molecular Formula: $C_7H_3F_3N_2O_4$

Molecular Weight: 236.107

Accurate Mass: 236.004492

Percentage Composition: C 35.61%; H 1.28%; F 24.14%; N 11.86%; O 27.11%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 49-50°

Aldrich: 19698-3

Fluka: 42026

Sigma: D0784

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 755B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1214B, (*ir*)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 830C, (*ir*)

Finger, G.C. *et al.*, *J.A.C.S.*, 1944, **66**, 1972, (*synth*)

Benkeser, R.A. *et al.*, *J.A.C.S.*, 1952, **74**, 3011, (*synth*)