



>>Entry Name: 1-Iodo-3-(trifluoromethyl)benzene, 9CI

Synonym(s): 3-Iodo- α,α,α -trifluorotoluene. 3-Iodobenzotrifluoride. α,α,α -Trifluoro-*m*-iodotoluene, 8CI

CAS Registry Number: 401-81-0

Molecular Formula: C₇H₄F₃I

Molecular Weight: 272.008

Accurate Mass: 271.930982

Percentage Composition: C 30.91%; H 1.48%; F 20.95%; I 46.65%

Physical Description: Yellow liq.

Boiling Point: Bp 182-183°. Bp₂₅ 82°

Aldrich: 20656-3

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **3**, 916B

Finger, G.C. *et al.*, *CA*, 1945, **39**, 1146, (*synth*)

Glennon, R.A. *et al.*, *J. Med. Chem.*, 1981, **24**, 678, (*synth*)

Naumann, D. *et al.*, *J. Fluorine Chem.*, 1990, **47**, 283, (*synth, F-19 nmr*)

Chambers, R.D. *et al.*, *J.C.S. Perkin 1*, 1996, 1659, (*synth, pmr, F-19 nmr, cmr*)