



>>Entry Name: 1-Iodooctane

Synonym(s): *n*-Octyl iodide

CAS Registry Number: 629-27-6

$\text{H}_3\text{C}(\text{CH}_2)_6\text{CH}_2\text{I}$

Molecular Formula: $\text{C}_8\text{H}_{17}\text{I}$

Molecular Weight: 240.127

Accurate Mass: 240.037498

Percentage Composition: C 40.02%; H 7.14%; I 52.85%

Physical Description: Liq.

Melting Point: Fp -45.7°

Boiling Point: Bp₅ 86.5°

Hazard & Toxicity: LD₅₀ (rat, ipr) 1982 mg/kg. Flammable, fl. p. 46°

Aldrich: 23829-5

Fluka: 57971

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 88C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 60B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 88A, (*ir*)

Vogel, A.I., *J.C.S.*, 1943, 636, (*synth*)

San Filippo, J. Jr. *et al.*, *J.A.C.S.*, 1975, **97**, 2546, (*pmr*)

Houriet, R. *et al.*, *Helv. Chim. Acta*, 1976, **59**, 119, (*ms*)

King, J.F. *et al.*, *J.A.C.S.*, 1978, **100**, 1637, (*synth*)