



>>Entry Name: 1-Iodoheptane, 9CI, 8CI

Synonym(s): *n*-Heptyl iodide

CAS Registry Number: 4282-40-0

$\text{H}_3\text{C}(\text{CH}_2)_5\text{CH}_2\text{I}$

Molecular Formula: $\text{C}_7\text{H}_{15}\text{I}$

Molecular Weight: 226.1

Accurate Mass: 226.021848

Percentage Composition: C 37.19%; H 6.69%; I 56.13%

Use/Importance: Reagent used in gc anal. of acetaminophen (paracetamol)

Physical Description: Liq.

Boiling Point: Bp 204°. Bp₁₇ 91°

Density: d_4^{20} 1.3774

Hazard & Toxicity: Fl. p. 79°

Aldrich: 17785-7

Fluka: 57870

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 87C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 59C, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 87B, (ir)

Sherrill, M.L., *J.A.C.S.*, 1930, **52**, 1982, (synth)

Corey, E.J. *et al.*, *J.O.C.*, 1967, **32**, 4160, (synth)

Dechtiaruk, W.A. *et al.*, *Clin. Chem. (Winston-Salem, N.C.)*, 1976, **22**, 879, (use)

Stahl, D. *et al.*, *Org. Mass Spectrom.*, 1977, **12**, 761, (ms)

Gavrilenko, V.V. *et al.*, *Zh. Obshch. Khim.*, 1978, **48**, 2073, (synth)