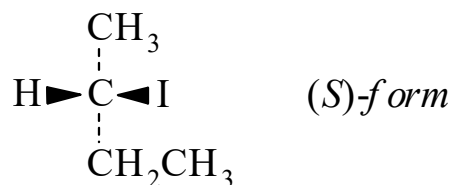




>>Entry Name: 2-Iodobutane, 9CI, 8CI

Synonym(s): *sec*-Butyl iodide



CAS Registry Number: 513-48-4

Molecular Formula: C₄H₉I

Molecular Weight: 184.02

Accurate Mass: 183.974898

Percentage Composition: C 26.11%; H 4.93%; I 68.96%

Hazard & Toxicity: Exp. neoplastic agent. Highly flammable, fl. p. -10/21°

Aldrich: 24432-5

Fluka: 20040

Rare Chemicals Library: S55798-6

>>Variant: (S)-form

CAS Registry Number: 29882-56-2

Molecular Formula: C₄H₉I

Molecular Weight: 184.02

Accurate Mass: 183.974898

Percentage Composition: C 26.11%; H 4.93%; I 68.96%

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{Hg}}^{24} +10.95$

>>Variant: (R)-form

CAS Registry Number: 22156-92-9

Molecular Formula: C₄H₉I

Molecular Weight: 184.02

Accurate Mass: 183.974898

Percentage Composition: C 26.11%; H 4.93%; I 68.96%

Physical Description: Oil

Boiling Point: Bp 118° (121-122°)

Optical Rotation: $[\alpha]_{\text{D}}^{24} -15.9$ (neat). $[\alpha]_{\text{D}}^{20} -10.77$ (neat)

Density: $d_4^{20} 1.58516$

>>Variant: (±)-form

CAS Registry Number: 52152-71-3

Molecular Formula: C₄H₉I

Molecular Weight: 184.02

Accurate Mass: 183.974898

Percentage Composition: C 26.11%; H 4.93%; I 68.96%

Physical Description: Liq., rapidly turning brown in light

Melting Point: Fp -104°

Boiling Point: Bp 119-120°. Bp₄₅ 33°

Density: $d_4^{20} 1.592$

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 97C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 66D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 95A, (*ir*)

Kenyon, J. *et al.*, *J.C.S.*, 1935, 1072

Levene, P.A. *et al.*, *J. Biol. Chem.*, 1936, **115**, 415, (*synth*)

Long, L.H. *et al.*, *Chem. Ind. (London)*, 1965, 223, (*synth*)

Meyers, A.I. *et al.*, *J.A.C.S.*, 1976, **98**, 2290, (*resoln*)

Kauffmann, T. *et al.*, *Angew. Chem., Int. Ed.*, 1977, **16**, 709, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, IEH000