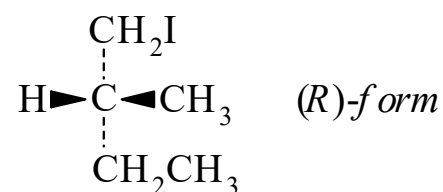




>>Entry Name: 1-Iodo-2-methylbutane, 9CI, 8CI
Synonym(s): *ac*-Amyl iodide. 2-Methylbutyl iodide



CAS Registry Number: 616-14-8

Molecular Formula: C₅H₁₁I
Molecular Weight: 198.046
Accurate Mass: 197.990548
Percentage Composition: C 30.32%; H 5.60%; I 64.08%

>>Variant: (*R*)-form

CAS Registry Number: 87106-25-0
Molecular Formula: C₅H₁₁I
Molecular Weight: 198.046
Accurate Mass: 197.990548
Percentage Composition: C 30.32%; H 5.60%; I 64.08%
Boiling Point: Bp 148°
Optical Rotation: $[\alpha]_{\text{D}}^{20} -5.96$ (c, 2.05 in CHCl₃)

>>Variant: (*S*)-form

CAS Registry Number: 29394-58-9
Molecular Formula: C₅H₁₁I
Molecular Weight: 198.046
Accurate Mass: 197.990548
Percentage Composition: C 30.32%; H 5.60%; I 64.08%
Physical Description: Liq.
Boiling Point: Bp 148°
Optical Rotation: $[\alpha]_{\text{D}}^{26} +6.1$ (c, 2.27 in CHCl₃) (prob. >99% ee). $[\alpha]_{\text{D}}^{20} +5.8$ (c, 7 in CH₂Cl₂)
Density: $d_4^{20} 1.524$
Refractive Index: $n_{\text{D}}^{14} 1.4966$
Aldrich: 32713-1
Sigma: I0762

>>Variant: ($\pm$)-form

Molecular Formula: C₅H₁₁I
Molecular Weight: 198.046
Accurate Mass: 197.990548
Percentage Composition: C 30.32%; H 5.60%; I 64.08%
Physical Description: Liq.
Boiling Point: Bp 143-144°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 101A, (*nmr*)
Klages, A. *et al.*, *Ber.*, 1904, **37**, 649, (*synth*)
Berlak, M.C. *et al.*, *J.C.S.*, 1949, 2309, (*synth*)
Inoue, S. *et al.*, *J. Organomet. Chem.*, 1970, **25**, 1, (*synth*)
Olah, G.A. *et al.*, *Synthesis*, 1974, 653, (*synth*)
Mori, C. *et al.*, *Annalen*, 1991, 213, (*synth*, *pmr*)
Martischonok, V. *et al.*, *Synthesis*, 1991, 560, (*synth*)
Takikawa, H. *et al.*, *Annalen*, 1996, 1965, (*synth*, *ir*, *pmr*)