



>>Entry Name: 4-Iodobutanoic acid, 9CI

Synonym(s): 4-Iodobutyric acid, 8CI

CAS Registry Number: 7425-27-6

ICH₂CH₂CH₂COOH

Molecular Formula: C₄H₇IO₂

Molecular Weight: 214.003

Accurate Mass: 213.949078

Percentage Composition: C 22.45%; H 3.30%; I 59.30%; O 14.95%

Physical Description: Cryst. (petrol)

Melting Point: Mp 40-41°

Solubility: Spar. sol. H₂O

Aldrich: 45356-0

>>Derivative: Me ester

CAS Registry Number: 14273-85-9

Molecular Formula: C₅H₉IO₂

Molecular Weight: 228.029

Accurate Mass: 227.964728

Percentage Composition: C 26.34%; H 3.98%; I 55.65%; O 14.03%

Physical Description: Liq.

Boiling Point: Bp 198-200°

Density: d⁵ 1.666

Aldrich: 46215-2

>>Derivative: Et ester

CAS Registry Number: 7425-53-8

Molecular Formula: C₆H₁₁IO₂

Molecular Weight: 242.056

Accurate Mass: 241.980378

Percentage Composition: C 29.77%; H 4.58%; I 52.43%; O 13.22%

Physical Description: Liq.

Boiling Point: Bp₁₃ 97°. Bp₄ 84-85°

Refractive Index: n_D²⁰ 1.4974

>>Derivative: Iodide

Molecular Formula: C₄H₆I₂O

Molecular Weight: 323.9

Accurate Mass: 323.850811

Percentage Composition: C 14.83%; H 1.87%; I 78.36%; O 4.94%

Physical Description: Bright yellow liq.

Boiling Point: Bp₂ 100°

References:

Fuson, R.C. *et al.*, *J.A.C.S.*, 1938, **60**, 2272-2273, (*Et ester*)

Blicke, F.F. *et al.*, *J.A.C.S.*, 1941, **63**, 2488-2490, (*synth, Et ester*)

Hauptmann, S. *et al.*, *J. Prakt. Chem.*, 1966, **34**, 262

Olah, G.A. *et al.*, *J.O.C.*, 1979, **44**, 1247, (*synth*)

Olah, G.A. *et al.*, *Synthesis*, 1982, 963, (*synth*)

Keinan, E. *et al.*, *J.O.C.*, 1990, **55**, 3922, (*iodide*)

Xu, Y.-C. *et al.*, *Can. J. Chem.*, 1993, **71**, 1152, (*Me ester, synth, ir*)