



>>Entry Name: 4-Nitrobutanoic acid

CAS Registry Number: 16488-43-0

O2NCH2CH2CH2COOH

Molecular Formula: C4H7NO4

Molecular Weight: 133.104

Accurate Mass: 133.037509

Percentage Composition: C 36.10%; H 5.30%; N 10.52%; O 48.08%

Physical Description: Oil

Boiling Point: Bp_{0.04} 120°

Refractive Index: n_D^{20.5} 1.4552

>>Derivative: Benzylamine salt

Melting Point: Mp 106°

>>Derivative: Me ester

CAS Registry Number: 13013-02-0

Molecular Formula: C5H9NO4

Molecular Weight: 147.13

Accurate Mass: 147.053159

Percentage Composition: C 40.82%; H 6.17%; N 9.52%; O 43.50%

Physical Description: Pale yellow liq.

Boiling Point: Bp_{0.25} 74-82°

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 110106-95-1

Molecular Formula: C8H15NO4

Molecular Weight: 189.211

Accurate Mass: 189.100109

Percentage Composition: C 50.78%; H 7.99%; N 7.40%; O 33.82%

Physical Description: Oil

Boiling Point: Bp₈ 111-113°. Bp_{0.2} 54-58°

>>Derivative: Chloride

CAS Registry Number: 75938-95-3

Molecular Formula: C4H6ClNO3

Molecular Weight: 151.549

Accurate Mass: 151.003621

Percentage Composition: C 31.70%; H 3.99%; Cl 23.39%; N 9.24%; O 31.67%

Physical Description: Pale yellow oil

Boiling Point: Bp_{0.03} 61-63°

References:

Seebach, D. *et al.*, *Helv. Chim. Acta*, 1981, **64**, 716, (*synth*)

Fuji, M. *et al.*, *Chem. Pharm. Bull.*, 1992, **40**, 2338, (*ester, chloride*)

Drinan, M.A. *et al.*, *J. Het. Chem.*, 1994, **31**, 255, (*synth*)

Bobal, P. *et al.*, *J. Het. Chem.*, 2001, **38**, 527-530, (*Me ester*)