



**>>Entry Name: 3-(4-Nitrophenyl)propanoic acid**

**Synonym(s):** 4-Nitrobenzenepropanoic acid, 9Cl. 3-(*p*-Nitrophenyl)propionic acid, 8Cl. *p*-Nitrohydrocinnamic acid

**CAS Registry Number:** 16642-79-8

**Molecular Formula:** C<sub>9</sub>H<sub>9</sub>NO<sub>4</sub>

**Molecular Weight:** 195.174

**Accurate Mass:** 195.053159

**Percentage Composition:** C 55.39%; H 4.65%; N 7.18%; O 32.79%

**Physical Description:** Needles (H<sub>2</sub>O)

**Melting Point:** Mp 163-164°

**pKa Value:** pK<sub>a1</sub> 4.54 (25°)

**>>Derivative:** Et ester

**CAS Registry Number:** 7116-34-9

**Molecular Formula:** C<sub>11</sub>H<sub>13</sub>NO<sub>4</sub>

**Molecular Weight:** 223.228

**Accurate Mass:** 223.084459

**Percentage Composition:** C 59.19%; H 5.87%; N 6.27%; O 28.67%

**Physical Description:** Cryst. (EtOH)

**Melting Point:** Mp 33-34°

**>>Derivative:** Amide

**CAS Registry Number:** 98953-18-5

**Molecular Formula:** C<sub>9</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>

**Molecular Weight:** 194.19

**Accurate Mass:** 194.069143

**Percentage Composition:** C 55.67%; H 5.19%; N 14.43%; O 24.72%

**Physical Description:** Needles (H<sub>2</sub>O)

**Melting Point:** Mp 174-175°

**>>Derivative:** Nitrile

**Synonym(s):** 1-Cyano-2-(4-nitrophenyl)ethane

**CAS Registry Number:** 53563-09-0

**Molecular Formula:** C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>

**Molecular Weight:** 176.174

**Accurate Mass:** 176.058578

**Percentage Composition:** C 61.36%; H 4.58%; N 15.90%; O 18.16%

**Physical Description:** Cryst.

**Melting Point:** Mp 79°

**References:**

Beilstein, F. *et al.*, *Annalen*, 1872, **163**, 121-143, (*synth*)

Zemplen, G. *et al.*, *Ber.*, 1928, **61**, 2486-2497, (*synth*)

Bowie, J.H. *et al.*, *Org. Mass Spectrom.*, 1977, **12**, 436-438, (*ms*)

Tóth, G. *et al.*, *Synth. Commun.*, 1995, **25**, 3067-3074, (*synth*)

Strazzolini, P. *et al.*, *J.O.C.*, 1998, **63**, 952-958, (*synth*, *nitrile*, *ir*, *pmr*, *cmr*, *ms*)

Moloney, G.P. *et al.*, *J. Med. Chem.*, 1999, **42**, 2504-2526, (*synth*)