



>>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: C₉H₉NO₄

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 (H₂O)

Melting Point: Mp 163-164°

pKa Value: pK_{a1} 4.54 (25°)

>>Derivative: Et ester

CAS Registry Number: 7116-34-9

Molecular Formula: C₁₁H₁₃NO₄

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: C₉H₁₀N₂O₃

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 (H₂O)

Melting Point: Mp 174-175°

>>Derivative: Nitrile

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

CAS Registry Number: 53563-09-0

Molecular Formula: C₉H₈N₂O₂

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*)