



>>Entry Name: 2-(4-Nitrophenyl)butanoic acid

Synonym(s): α -Ethyl-4-nitrobenzeneacetic acid, 9Cl. 2-(*p*-Nitrophenyl)butyric acid, 8Cl

CAS Registry Number: 7463-53-8

Molecular Formula: C₁₀H₁₁NO₄

Molecular Weight: 209.201

Accurate Mass: 209.068809

Percentage Composition: C 57.41%; H 5.30%; N 6.70%; O 30.59%

Hazard & Toxicity: LD₅₀ (mus, ipr) 240 mg/kg

>>Variant: (+)-form

Molecular Formula: C₁₀H₁₁NO₄

Molecular Weight: 209.201

Accurate Mass: 209.068809

Percentage Composition: C 57.41%; H 5.30%; N 6.70%; O 30.59%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 120-122°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +17.7$ (EtOAc)

>>Variant: (±)-form

CAS Registry Number: 25227-34-3

Molecular Formula: C₁₀H₁₁NO₄

Molecular Weight: 209.201

Accurate Mass: 209.068809

Percentage Composition: C 57.41%; H 5.30%; N 6.70%; O 30.59%

Physical Description: Pale-yellow plates (C₆H₆)

Melting Point: Mp 121-122.5°

>>Derivative: Et ester

CAS Registry Number: 6973-78-0

Molecular Formula: C₁₂H₁₅NO₄

Molecular Weight: 237.255

Accurate Mass: 237.100109

Percentage Composition: C 60.75%; H 6.37%; N 5.90%; O 26.97%

Physical Description: Pale-yellow liq.

Boiling Point: Bp_{0.01} 93-94°

References:

Chu, T. *et al.*, *J.A.C.S.*, 1933, **55**, 2841, (*synth*)

Wilds, A.L. *et al.*, *J.A.C.S.*, 1945, **67**, 789, (*synth*)