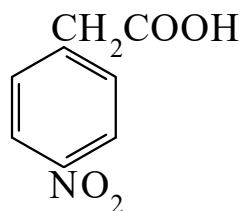




>>Entry Name: (4-Nitrophenyl)acetic acid

Synonym(s): 4-Nitrobenzeneacetic acid, gCl



CAS Registry Number: 104-03-0

Molecular Formula: C₈H₇NO₄

Molecular Weight: 181.148

Accurate Mass: 181.037509

Percentage Composition: C 53.04%; H 3.89%; N 7.73%; O 35.33%

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 153° (150°)

pKa Value: pK_{a1} 3.92 (25°)

Aldrich: N2020-4

Fluka: 73650

Sigma: N9251

>>Derivative: Me ester

CAS Registry Number: 2945-08-6

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 (petrol)

Melting Point: Mp 54°

Rare Chemicals Library: S59560-8

>>Derivative: Et ester

CAS Registry Number: 5445-26-1

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: Leaflets (petrol)

Melting Point: Mp 65.5-66°

Boiling Point: Bp₂₀ 196-197°

Rare Chemicals Library: S56014-6

>>Derivative: Chloride

CAS Registry Number: 50434-36-1

Molecular Formula: C₈H₆ClNO₃

Molecular Weight: 199.593

Accurate Mass: 199.003621

Percentage Composition: C 48.14%; H 3.03%; Cl 17.76%; N 7.02%; O 24.05%

Physical Description: Pale-yellow plates (petrol)

Melting Point: Mp 46-47°

Aldrich: 46249-7

>>Derivative: Amide

CAS Registry Number: 6321-12-6

Molecular Formula: C₈H₈N₂O₃

Molecular Weight: 180.163

Accurate Mass: 180.053493

Percentage Composition: C 53.33%; H 4.48%; N 15.55%; O 26.64%

Physical Description: Prisms

Melting Point: Mp 197-198° (191°)