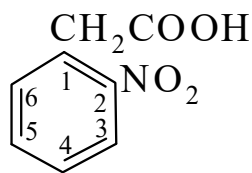




>>Entry Name: (2-Nitrophenyl)acetic acid

Synonym(s): 2-Nitrobenzeneacetic acid, 9CI



CAS Registry Number: 3740-52-1

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 (EtOH)

Melting Point: Mp 141-142.5°

Aldrich: 13024-9

Fluka: 73648

Sigma: N0631

>>Derivative: Me ester

CAS Registry Number: 30095-98-8

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: Liq.

Boiling Point: Bp 264°

>>Derivative: Et ester

CAS Registry Number: 31912-02-4

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-cream needles (EtOH)

Melting Point: Mp 69°

Rare Chemicals Library: S80921-7

>>Derivative: Chloride

CAS Registry Number: 22751-23-1

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%

Hazard & Toxicity: Can explode on isolation. Use in soln. recommended

>>Derivative: Amide

CAS Registry Number: 31142-60-6

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: Leaflets or needles (C₆H₆ or EtOH)

Melting Point: Mp 160-161°

>>Derivative: Nitrile

Synonym(s): *o*-Nitrobenzyl cyanide