



>>Entry Name: (3-Nitrophenyl)acetic acid

Synonym(s): 3-Nitrobenzeneacetic acid, gCl

CAS Registry Number: 1877-73-2

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 120° (117-118°)

pKa Value: pK_{a1} 3.95 (25°)

Aldrich: 10360-8

Fluka: 73647

Sigma: N4257

>>Derivative: Me ester

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: Waxy needles

Melting Point: Mp 28-30°

>>Derivative: Amide

CAS Registry Number: 5247-25-6

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: Cryst. (H₂O)

Melting Point: Mp 109-110°

>>Derivative: Nitrile

Synonym(s): *m*-Nitrobenzyl cyanide

CAS Registry Number: 621-50-1

Molecular Formula: C₈H₆N₂O₂

Molecular Weight: 162.148

Accurate Mass: 162.042928

Percentage Composition: C 59.26%; H 3.73%; N 17.28%; O 19.73%

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 61-62°

Aldrich: 37793-7

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1010B, (*nmr*)

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Bowie, J.H. *et al.*, *Org. Mass Spectrom.*, 1976, **11**, 1105, (*ms*)

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