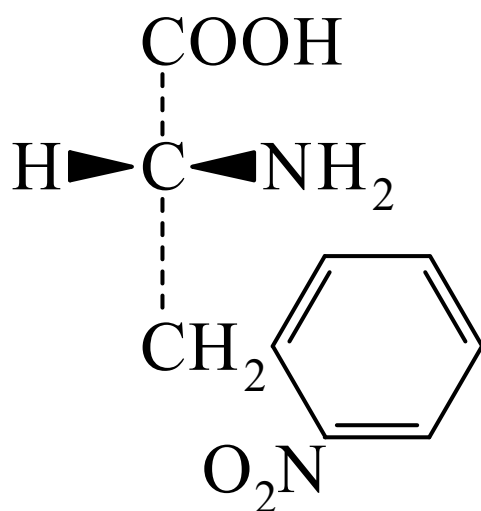




>>Entry Name: 2-Amino-3-(2-nitrophenyl)propanoic acid

Synonym(s): 3-(2-Nitrophenyl)alanine, 9CI. α -Amino-2-nitrobenzenepropanoic acid



(*R*)-form

Related CAS Registry Numbers(s): 19883-75-1 35987-87-2 164648-12-8 169383-17-9

Molecular Formula: $C_9H_{10}N_2O_4$

Molecular Weight: 210.189

Accurate Mass: 210.064058

Percentage Composition: C 51.43%; H 4.80%; N 13.33%; O 30.45%

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 35987-86-1

Molecular Formula: $C_9H_{10}N_2O_4$

Molecular Weight: 210.189

Accurate Mass: 210.064058

Percentage Composition: C 51.43%; H 4.80%; N 13.33%; O 30.45%

Physical Description: Cryst. (MeOH/Et₂O) (as hydrochloride)

Melting Point: Mp 223-224 dec.° (hydrochloride)

Optical Rotation: $[\alpha]_D^{21} -16.5$ (c, 0.5 in H₂O)

Other Data: CAS no. refers to hydrochloride

>>Derivative: *N*-Ac

CAS Registry Number: 35987-84-9

Molecular Formula: $C_{11}H_{12}N_2O_5$

Molecular Weight: 252.226

Accurate Mass: 252.074623

Percentage Composition: C 52.38%; H 4.80%; N 11.11%; O 31.72%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 202°

Optical Rotation: $[\alpha]_D^{21} -42$ (c, 1 in MeOH)

>>Variant: ($\pm$)-form

CAS Registry Number: 35378-63-3

Molecular Formula: $C_9H_{10}N_2O_4$

Molecular Weight: 210.189

Accurate Mass: 210.064058

Percentage Composition: C 51.43%; H 4.80%; N 13.33%; O 30.45%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 226-227 dec.°

References:

Weichert, R., *Annalen*, 1963, **662**, 160, (*synth*)

Davis, A.L. *et al.*, *J. Med. Chem.*, 1972, **15**, 325, (*synth*)