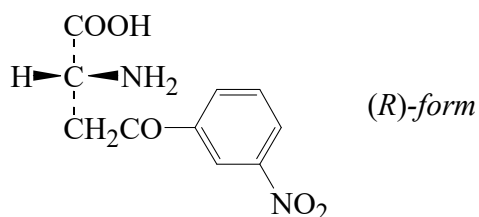




>>Entry Name: α -Amino-3-nitro- γ -oxobenzenebutanoic acid, 9CI

Synonym(s): (*m*-Nitrobenzoyl)alanine



Molecular Formula: C₁₀H₁₀N₂O₅

Molecular Weight: 238.199

Accurate Mass: 238.058973

Percentage Composition: C 50.42%; H 4.23%; N 11.76%; O 33.58%

Biological Use/Importance: Selective inhibitor of kynurenine-3-hydroxylase. Anticonvulsant agent

>>Variant: (*R*)-form

CAS Registry Number: 167819-02-5

Molecular Formula: C₁₀H₁₀N₂O₅

Molecular Weight: 238.199

Accurate Mass: 238.058973

Percentage Composition: C 50.42%; H 4.23%; N 11.76%; O 33.58%

>>Derivative: Hydrochloride

Optical Rotation: [α]_D²²−14.7 (c, 0.5 in H₂O)

>>Variant: (*S*)-form

CAS Registry Number: 167819-00-3

Molecular Formula: C₁₀H₁₀N₂O₅

Molecular Weight: 238.199

Accurate Mass: 238.058973

Percentage Composition: C 50.42%; H 4.23%; N 11.76%; O 33.58%

Other Data: Pharmacol. active isomer

>>Derivative: Hydrochloride

Melting Point: Mp 196-197°

Optical Rotation: [α]_D²²+13.21 (c, 1.0 in H₂O)

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

CAS Registry Number: 153212-71-6

Molecular Formula: C₁₀H₁₀N₂O₅

Molecular Weight: 238.199

Accurate Mass: 238.058973

Percentage Composition: C 50.42%; H 4.23%; N 11.76%; O 33.58%

Melting Point: Mp 187-188°

References:

- Pellicciari, R. *et al.*, *J. Med. Chem.*, 1994, **37**, 647-655, (*synth, pharmacol*)
Carpenedo, R. *et al.*, *Neurosci. (Oxford)*, 1994, **61**, 237-244, (*pharmacol*)
Natalini, B. *et al.*, *Bioorg. Med. Chem. Lett.*, 1995, **5**, 1451-1454, (*isomers, synth*)
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