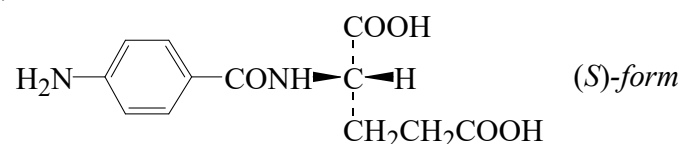




>>Entry Name: *N*-(4-Aminobenzoyl)glutamic acid, 9Cl



CAS Registry Number: 532-63-8

Molecular Formula: C₁₂H₁₄N₂O₅

Molecular Weight: 266.253

Accurate Mass: 266.090273

Percentage Composition: C 54.13%; H 5.30%; N 10.52%; O 30.05%

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 5959-18-2

Molecular Formula: C₁₂H₁₄N₂O₅

Molecular Weight: 266.253

Accurate Mass: 266.090273

Percentage Composition: C 54.13%; H 5.30%; N 10.52%; O 30.05%

Physical Description: Microscopic needles (H₂O)

Melting Point: Mp 166-167°

>>Variant: (*S*)-form

Synonym(s): L-form

CAS Registry Number: 4271-30-1

Molecular Formula: C₁₂H₁₄N₂O₅

Molecular Weight: 266.253

Accurate Mass: 266.090273

Percentage Composition: C 54.13%; H 5.30%; N 10.52%; O 30.05%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 172-173° (169-170°)

Optical Rotation: [α]_D²² +29.2 (1*M* NaOH)

pKa Value: p*K*_{a1} 4.83; p*K*_{a2} 3.76 (23.5°, 1*M* KCl)

Sigma: A0879

Other: PB A18200

>>Derivative: Hydrochloride

CAS Registry Number: 82683-96-3

Physical Description: Thin spear-shaped cryst. (HCl aq.)

Melting Point: Mp 197-198°

>>Derivative: Di-Me ester

CAS Registry Number: 52407-60-0

Molecular Formula: C₁₄H₁₈N₂O₅

Molecular Weight: 294.307

Accurate Mass: 294.121573

Percentage Composition: C 57.14%; H 6.16%; N 9.52%; O 27.18%

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 110-112.5°

>>Derivative: 5-Et ester

Molecular Formula: C₁₄H₁₈N₂O₅

Molecular Weight: 294.307

Accurate Mass: 294.121573

Percentage Composition: C 57.14%; H 6.16%; N 9.52%; O 27.18%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 128-129°