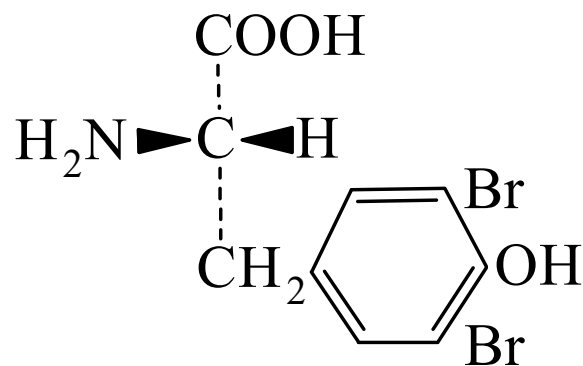




>>Entry Name: 2-Amino-3-(3,5-dibromo-4-hydroxyphenyl)propanoic acid

Synonym(s): 3,5-Dibromotyrosine



CAS Registry Number: 537-24-6

Molecular Formula: C₉H₉Br₂NO₃

Molecular Weight: 338.983

Accurate Mass: 336.934916

Percentage Composition: C 31.89%; H 2.68%; Br 47.14%; N 4.13%; O 14.16%

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 300-38-9

Molecular Formula: C₉H₉Br₂NO₃

Molecular Weight: 338.983

Accurate Mass: 336.934916

Percentage Composition: C 31.89%; H 2.68%; Br 47.14%; N 4.13%; O 14.16%

Biological Source: Isol. from sponges and gorgonians

Melting Point: Mp 245°

Sigma: D5632

>>Derivative: N-Ac

Molecular Formula: C₁₁H₁₁Br₂NO₄

Molecular Weight: 381.02

Accurate Mass: 378.945481

Percentage Composition: C 34.68%; H 2.91%; Br 41.94%; N 3.68%; O 16.80%

Use/Importance: Resolving agent

Physical Description: Cryst. + ½ H₂O (MeOH aq.)

Melting Point: Mp 118°

Optical Rotation: [α]_D²⁵ +34.5 (c, 4 in MeOH)

>>Variant: (±)-form

CAS Registry Number: 5741-93-5

Molecular Formula: C₉H₉Br₂NO₃

Molecular Weight: 338.983

Accurate Mass: 336.934916

Percentage Composition: C 31.89%; H 2.68%; Br 47.14%; N 4.13%; O 14.16%

>>Derivative: N-Ac

Molecular Formula: C₁₁H₁₁Br₂NO₄

Molecular Weight: 381.02

Accurate Mass: 378.945481

Percentage Composition: C 34.68%; H 2.91%; Br 41.94%; N 3.68%; O 16.80%

Melting Point: Mp 213-215 dec.°

>>Variant: (ξ)-form

Molecular Formula: C₉H₉Br₂NO₃

Molecular Weight: 338.983

Accurate Mass: 336.934916

Percentage Composition: C 31.89%; H 2.68%; Br 47.14%; N 4.13%; O 14.16%