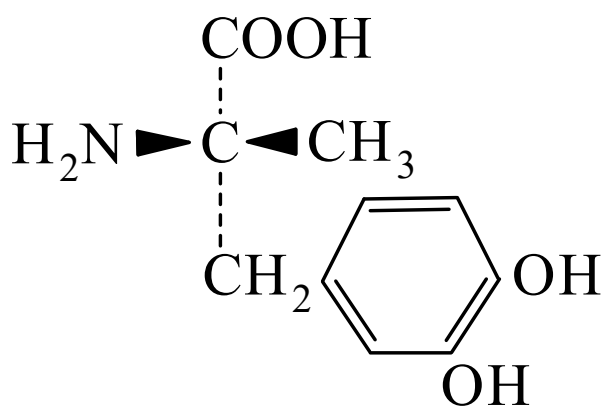




>>Entry Name: 2-Amino-3-(3,4-dihydroxyphenyl)-2-methylpropanoic acid

Synonym(s): 3-Hydroxy- α -methyltyrosine, 9Cl. 3-(3,4-Dihydroxyphenyl)-2-methylalanine, 8Cl. α -Amino-3,4-dihydroxy- α -methylhydrocinnamic acid. α -Methyl-3,4-dihydroxyphenylalanine. α -Methyldopa



CAS Registry Number: 55-40-3

Related CAS Registry Numbers(s): 555-29-3 2544-09-4 5123-53-5 41372-08-1

Molecular Formula: C₁₀H₁₃NO₄

Molecular Weight: 211.217

Accurate Mass: 211.084459

Percentage Composition: C 56.87%; H 6.20%; N 6.63%; O 30.30%

Use/Importance: Centrally acting antihypertensive agent

Calculated Log P Data: Log P -2.11 (uncertain value) (calc)

Hazard & Toxicity: Human systemic effects, incl. drowsiness, reported when used therapeutically. Human and exp. reprod. effects

>>Variant: (S)-form

Synonym(s): L-form. **Methyldopa**, BAN, INN, USAN. Aldomet. Dopamet. Hydromet. Medomet. Many other names

CAS Registry Number: 555-30-6

Molecular Formula: C₁₀H₁₃NO₄

Molecular Weight: 211.217

Accurate Mass: 211.084459

Percentage Composition: C 56.87%; H 6.20%; N 6.63%; O 30.30%

Use/Importance: Used as 0.07M soln. in isopropanol for fluorimetric detn. of Tb(III) ($\lambda_{\max}$ 530-560 nm; pH 9.8-10.0)

Physical Description: Cryst. + 1/2 H₂O (H₂O), cryst. + 3/2 H₂O (0.5% H₂SO₃), powder (anhyd.)

Melting Point: Mp 306-307 dec.°

Optical Rotation: $[\alpha]_D^{25}$ -5.2 (c, 2.0 in 0.1M HCl). $[\alpha]_D^{20}$ -14 (c, 1.09 in H₂)

Solubility: Sol. isopropanol, EtOH, H₂O; prac. insol. most org. solvs.

Fluka: 37862

Sigma: M0761

>>Derivative: Et ester

Synonym(s): **Methyldopate**, BAN

CAS Registry Number: 6014-30-8

Molecular Formula: C₁₂H₁₇NO₄

Molecular Weight: 239.271

Accurate Mass: 239.115759

Percentage Composition: C 60.24%; H 7.16%; N 5.85%; O 26.75%

Use/Importance: Antihypertensive agent

Physical Description: Amorph.

Optical Rotation: $[\alpha]_D$ -10 (c, 1 in 1M HCl)

Calculated Log P Data: Log P 0.55 (calc)

>>Derivative: Et ester; hydrochloride

Synonym(s): **Methyldopate hydrochloride**, USAN

CAS Registry Number: 2508-79-4

Physical Description: Cryst.

References: