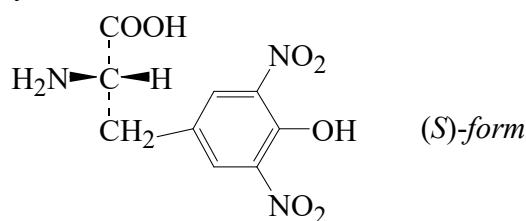




>>Entry Name: 2-Amino-3-(4-hydroxy-3,5-dinitrophenyl)propanoic acid

Synonym(s): 3,5-Dinitrotyrosine. 4-Hydroxy-3,5-dinitrophenylalanine



CAS Registry Number: 18386-16-8

Related CAS Registry Numbers(s): 71876-87-4

Molecular Formula: C₉H₉N₃O₇

Molecular Weight: 271.186

Accurate Mass: 271.044052

Percentage Composition: C 39.86%; H 3.34%; N 15.49%; O 41.30%

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 17360-11-1

Extra CAS Registry Numbers(s): 71876-88-5

Molecular Formula: C₉H₉N₃O₇

Molecular Weight: 271.186

Accurate Mass: 271.044052

Percentage Composition: C 39.86%; H 3.34%; N 15.49%; O 41.30%

Physical Description: Yellow cryst. (H₂O)

Melting Point: Mp 230-232° (228-229°)(monohydrate)

Optical Rotation: $[\alpha]_D^{15} +11.45$ (c, 1.52 in 2M HCl)

Rare Chemicals Library: S40561-2

Sigma: D3130

Other: PB D48180

>>Derivative: Me ester

CAS Registry Number: 24788-04-3

Physical Description: Pale yellow needles (MeOH aq.) (as hydrochloride)

Optical Rotation: $[\alpha]_D^{20} -13.5$ (c, 1 in DMF) (hydrochloride)

Other Data: CAS no. refers to hydrochloride

>>Derivative: N-Ac

CAS Registry Number: 20767-00-4

Molecular Formula: C₁₁H₁₁N₃O₈

Molecular Weight: 313.223

Accurate Mass: 313.054617

Percentage Composition: C 42.18%; H 3.54%; N 13.42%; O 40.86%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 189-190°

Optical Rotation: $[\alpha]_D +12.2$ (c, 1.15 in dioxan)

Sigma: A7625

>>Derivative: N-Ac, Et ester

CAS Registry Number: 29358-99-4

Molecular Formula: C₁₃H₁₅N₃O₈

Molecular Weight: 341.277

Accurate Mass: 341.085917

Percentage Composition: C 45.75%; H 4.43%; N 12.31%; O 37.50%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 120-121°

Optical Rotation: $[\alpha]_D^{23} -6.75$ (c, 6.2 in dioxan)

Sigma: A7750