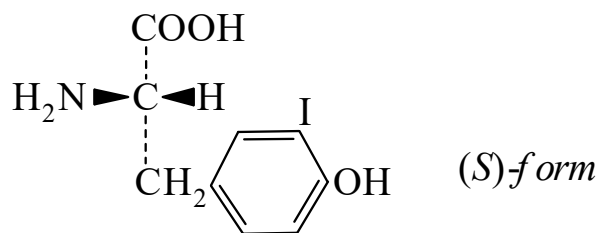




>>Entry Name: 2-Amino-3-(3-iodo-4-hydroxyphenyl)propanoic acid

Synonym(s): 3-Iodotyrosine, 9Cl. Monoiodotyrosine. Iotyrosine



Related CAS Registry Numbers(s): 16624-40-1 19254-01-4 20520-42-7 60345-92-8 70277-02-0 78758-99-3

Molecular Formula: C₉H₁₀INO₃

Molecular Weight: 307.087

Accurate Mass: 306.970542

Percentage Composition: C 35.20%; H 3.28%; I 41.33%; N 4.56%; O 15.63%

Use/Importance: ¹³¹I labelled cpd. is used as a radioactive agent

Calculated Log P Data: Log P -1.15 (uncertain value) (calc)

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 70-78-0

Molecular Formula: C₉H₁₀INO₃

Molecular Weight: 307.087

Accurate Mass: 306.970542

Percentage Composition: C 35.20%; H 3.28%; I 41.33%; N 4.56%; O 15.63%

Biological Source: Occurs in thyroid tissue and human blood serum. Prod. by sponges

Physical Description: Cryst. (H₂O)

Melting Point: Mp 202-204°

Optical Rotation: [α]_D²⁰ -4.4 (c, 5 in 1M HCl)

Solubility: Sol. hot H₂O

Aldrich: I-1180-1

Fluka: 58120

Sigma: I8250

>>Variant: (±)-form

Molecular Formula: C₉H₁₀INO₃

Molecular Weight: 307.087

Accurate Mass: 306.970542

Percentage Composition: C 35.20%; H 3.28%; I 41.33%; N 4.56%; O 15.63%

Physical Description: Cryst. + 1H₂O (H₂O)

Melting Point: Mp 200-201 dec.°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1189B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 256C, (ir)

Harington, C.R. *et al.*, *Biochem. J.*, 1944, **38**, 320, (synth)

Pitt-Rivers, R. *et al.*, *Chem. Ind. (London)*, 1956, 21, (synth)

Hillman, G. *et al.*, *Hoppe Seyler's Z. Physiol. Chem.*, 1956, **305**, 177, (synth)

Wynn, J., *Arch. Biochem. Biophys.*, 1960, **88**, 98

Bednar, J. *et al.*, *Radiochem. Radioanal. Lett.*, 1980, **45**, 377, (use)

Baron, M.H. *et al.*, *J. Chim. Phys. Phys.-Chim. Biol.*, 1983, **80**, 729, (Raman)

Okabe, N. *et al.*, *Acta Cryst. C*, 1995, **51**, 1700, (cryst struct)