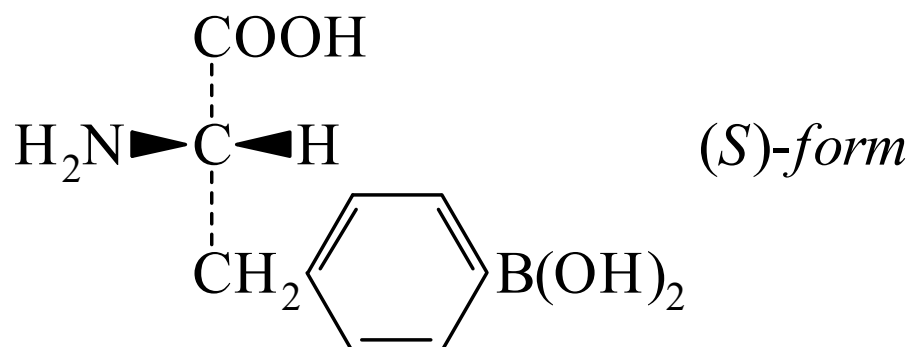




>>Entry Name: 2-Amino-3-(4-boronophenyl)propanoic acid

Synonym(s): 4-Boronophenylalanine, 9Cl



CAS Registry Number: 90580-64-6

Related CAS Registry Numbers(s): 74923-16-3 76410-59-8 80994-59-8 91196-68-8 111821-49-9

Molecular Formula: C₉H₁₂BNO₄

Molecular Weight: 209.009

Accurate Mass: 209.085939

Percentage Composition: C 51.72%; H 5.79%; B 5.17%; N 6.70%; O 30.62%

Use/Importance: ¹⁰B-labelled-form is used in boron neutron capture therapy

>>Variant: (S)-form

CAS Registry Number: 76410-58-7

Molecular Formula: C₉H₁₂BNO₄

Molecular Weight: 209.009

Accurate Mass: 209.085939

Percentage Composition: C 51.72%; H 5.79%; B 5.17%; N 6.70%; O 30.62%

Source/Synthesis: Synth. in 3 steps from Dihydroxy(4-iodophenyl)borane [NZT04-Y](#)

Physical Description: Cryst.

Melting Point: Mp 285-290°

Optical Rotation: [α]_D²³ −8.3 (c, 0.9 in 1M HCl)

>>Variant: (±)-form

CAS Registry Number: 77374-29-9

Molecular Formula: C₉H₁₂BNO₄

Molecular Weight: 209.009

Accurate Mass: 209.085939

Percentage Composition: C 51.72%; H 5.79%; B 5.17%; N 6.70%; O 30.62%

Physical Description: Cryst.

Melting Point: Mp 285-290 dec.°

>>Derivative: Hydrochloride

CAS Registry Number: 112725-17-4

Physical Description: Cryst.

Melting Point: Mp 200-203°

References:

Snyder, H.R. *et al.*, *J.A.C.S.*, 1958, **80**, 835, (*synth*)

Coderre, J.A. *et al.*, *Cancer Res.*, 1987, **47**, 6377, (*synth, use*)

Malan, C. *et al.*, *Synlett*, 1996, 167, (*synth, pmr, cmr, B-11 nmr*)

Park, K.C. *et al.*, *Synthesis*, 1999, 2041-2044, (*synth, ir, pmr, cmr, B-11 nmr*)

Nakamura, H. *et al.*, *Bull. Chem. Soc. Jpn.*, 2000, **73**, 231-235, (*S-form, synth, pmr*)