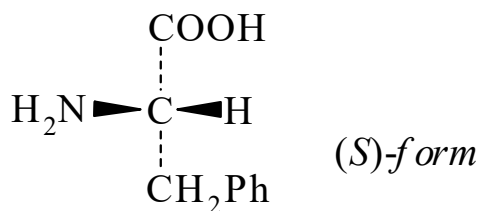




>>Entry Name: Phenylalanine, 9CI, USAN

ENTRY UNDER REVIEW

Synonym(s):  $\alpha$ -Aminobenzenepropanoic acid. 2-Amino-3-phenylpropanoic acid.  $\beta$ -Phenylalanine. FN 1636. Antibiotic FN 1636. Phe



CAS Registry Number: 3617-44-5

Related CAS Registry Numbers(s): 60058-39-1 65864-22-4

Molecular Formula:  $C_9H_{11}NO_2$

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Calculated Log P Data: Log P -1.56 (uncertain value) (calc)

>>Variant: (*R*)-form

Synonym(s): D-form

CAS Registry Number: 673-06-3

Molecular Formula:  $C_9H_{11}NO_2$

Molecular Weight: 165.191

Accurate Mass: 165.078979

Percentage Composition: C 65.44%; H 6.71%; N 8.48%; O 19.37%

Biological Source: Residue present in Islanditoxin [CKG27-C](#)

Physical Description: Leaflets ( $H_2O$ )

Melting Point: Mp 196 dec. $^{\circ}$ . Mp 283-284 dec. $^{\circ}$

Optical Rotation:  $[\alpha]_D^{25} +34.5$  (c, 1 in  $H_2O$ ).  $[\alpha]_D +4.47$  (c, 1 in 5M HCl)

Hazard & Toxicity: Human systemic effects by ingestion reported (gastrointestinal). LD<sub>50</sub> (rat, ipr) 5452 mg/kg

Aldrich: 16261-2

Fluka: 78030

Sigma: P1751

>>Derivative: Me ester

CAS Registry Number: 21685-51-8

Extra CAS Registry Numbers(s): 13033-84-6

Molecular Formula:  $C_{10}H_{13}NO_2$

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Physical Description: Liq.

Boiling Point: Bp<sub>0.1</sub> 95 $^{\circ}$

Optical Rotation:  $[\alpha]_D^{20} -26$  (c, 2.2 in EtOH) (>95% ee)

>>Derivative: Et ester

CAS Registry Number: 63060-94-6

Molecular Formula:  $C_{11}H_{15}NO_2$

Molecular Weight: 193.245

Accurate Mass: 193.110279

Percentage Composition: C 68.37%; H 7.82%; N 7.25%; O 16.56%

Physical Description: Cryst. (EtOH/Et<sub>2</sub>O) (as hydrochloride)

Melting Point: Mp 156-158 $^{\circ}$  (hydrochloride)

Optical Rotation:  $[\alpha]_D^{21} -36.5$  (c, 4.8 in EtOH)