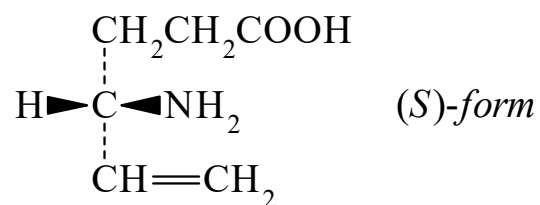




>>Entry Name: 4-Amino-5-hexenoic acid, 9CI

Synonym(s): Vigabatrin, BAN, INN, USAN. γ -Vinyl GABA. Sabril. GVG. MDL 71754. RMI 71754



CAS Registry Number: 60643-86-9

Related CAS Registry Numbers(s): 77162-51-7

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}_2$

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Use/Importance: Anticonvulsant. Inhibitor of GABA transaminase

Development Status: Launched 1989

Calculated Log P Data: Log P -2.98 (calc)

Sigma: V8261

>>Variant: (R)-form

CAS Registry Number: 77162-51-7

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}_2$

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Melting Point: Mp 164-165°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -12.2$ (c, 4.5 in H_2O)

>>Variant: (S)-form

CAS Registry Number: 74046-07-4

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}_2$

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Physical Description: Cryst. (EtOH/2-propanol)

Melting Point: Mp 207-209° (163-165°)

Optical Rotation: $[\alpha]_{\text{D}} +12.4$ (c, 0.5 in H_2O)

Other Data: Pharmacol. active isomer

>>Variant: ($\pm$)-form

CAS Registry Number: 68506-86-5

Molecular Formula: $\text{C}_6\text{H}_{11}\text{NO}_2$

Molecular Weight: 129.158

Accurate Mass: 129.078979

Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%

Physical Description: Cryst. (EtOH aq.)

References: