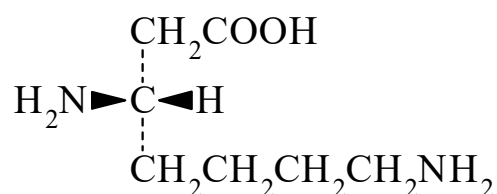




>>Entry Name: 3,7-Diaminoheptanoic acid, 9CI, 8CI



CAS Registry Number: 89687-33-2

Molecular Formula: C₇H₁₆N₂O₂

Molecular Weight: 160.216

Accurate Mass: 160.121178

Percentage Composition: C 52.48%; H 10.07%; N 17.48%; O 19.97%

>>Variant: (S)-form

CAS Registry Number: 13184-41-3

Molecular Formula: C₇H₁₆N₂O₂

Molecular Weight: 160.216

Accurate Mass: 160.121178

Percentage Composition: C 52.48%; H 10.07%; N 17.48%; O 19.97%

Physical Description: Gum

Optical Rotation: $[\alpha]_D^{21} +29$ (c, 1 in H₂O)

>>Derivative: Me ester

CAS Registry Number: 85120-14-5

Molecular Formula: C₈H₁₈N₂O₂

Molecular Weight: 174.242

Accurate Mass: 174.136828

Percentage Composition: C 55.15%; H 10.41%; N 16.08%; O 18.36%

Melting Point: Mp 118-119 dec.°

Optical Rotation: $[\alpha]_D^{22} -3$ (c, 2 in CHCl₃)

>>Derivative: 7-N-(tert-Butoxycarbonyl)-3-N-[(9H-fluoren-9-yl-methoxy)carbonyl]

CAS Registry Number: 203854-47-1

Molecular Formula: C₂₇H₃₄N₂O₆

Molecular Weight: 482.575

Accurate Mass: 482.241688

Percentage Composition: C 67.20%; H 7.10%; N 5.80%; O 19.89%

Physical Description: Cryst. (CHCl₃/hexane)

Melting Point: Mp 97 dec.°

Optical Rotation: $[\alpha]_D -8.3$ (c, 0.92 in CHCl₃)

References:

Yonehara, H. *et al.*, *Tet. Lett.*, 1966, 3785-3791, (*ord*)

Japan. Pat., 1982, 57 188 562; *CA*, **98**, 178765q, (*synth*)

Guichard, G. *et al.*, *Helv. Chim. Acta*, 1998, **81**, 187-206, (*deriv, synth, ir, pmr, cmr, ms*)