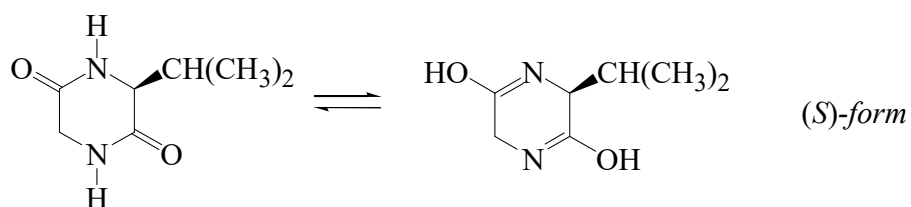




>>Entry Name: **3-Isopropyl-2,5-piperazinedione**

Synonym(s): 3-(1-Methylethyl)-2,5-piperazinedione, 9Cl. 3-Isopropyl-2,5-dioxopiperazine. Cyclo(glycylvalyl). Cyclo(valylglycyl). Glycylvaline anhydride. Valylglycine anhydride



Related CAS Registry Numbers(s): 109838-85-9 117457-09-7

Molecular Formula: C₇H₁₂N₂O₂

Molecular Weight: 156.184

Accurate Mass: 156.089878

Percentage Composition: C 53.83%; H 7.74%; N 17.94%; O 20.49%

>>Variant: (S)-form

CAS Registry Number: 16944-60-8

Molecular Formula: C₇H₁₂N₂O₂

Molecular Weight: 156.184

Accurate Mass: 156.089878

Percentage Composition: C 53.83%; H 7.74%; N 17.94%; O 20.49%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 264-265° (254°)

Optical Rotation: [α]_D²⁰+20.2 (c, 0.9 in H₂O)

>>Variant: (S)-Bislactim-form

Molecular Formula: C₇H₁₂N₂O₂

Molecular Weight: 156.184

Accurate Mass: 156.089878

Percentage Composition: C 53.83%; H 7.74%; N 17.94%; O 20.49%

>>Derivative: Di-Me ether

Synonym(s): 2,5-Dihydro-3,6-dimethoxy-2-(1-methylethyl)pyrazine, 9Cl

CAS Registry Number: 78342-42-4

Molecular Formula: C₉H₁₆N₂O₂

Molecular Weight: 184.238

Accurate Mass: 184.121178

Percentage Composition: C 58.67%; H 8.75%; N 15.21%; O 17.37%

Use/Importance: Undergoes enantioselective alkylation for the synth. of amino acids

Boiling Point: Bp₁₀ 88°

Optical Rotation: [α]_D²⁰+106.3 (c, 1.0 in EtOH)

References:

Kopple, K.D. *et al.*, *J.O.C.*, 1968, **33**, 862-864, (*synth*)

Kopple, K.D. *et al.*, *J.A.C.S.*, 1969, **91**, 962-970, (*pmr*)

Chandrasekaran, R. *et al.*, *Biopolymers*, 1973, **12**, 1421-1425, (*pmr, conformn*)

Schoellkopf, U. *et al.*, *Angew. Chem., Int. Ed.*, 1981, **20**, 798-799, (*synth, use, deriv*)

Schoellkopf, U., *Tetrahedron*, 1983, **39**, 2089-2091, (*use, deriv*)