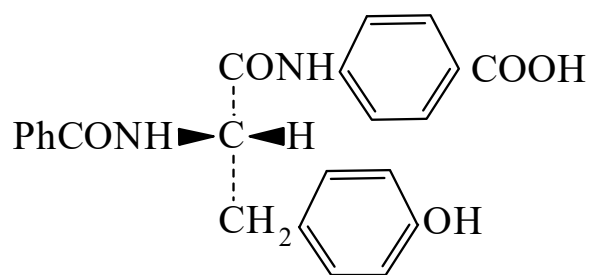




>>Entry Name: Bentiromide, BAN, INN, JAN, USAN

Synonym(s): 4-[[2-(Benzoylamino)-3-(4-hydroxyphenyl)-1-oxopropyl]amino]benzoic acid, 9Cl. 4-(N-Benzoyltyrosylamino)benzoic acid. Bentirosin. Chymex. Exocrine. E 2663. Ro 11-7891. PFD



Molecular Formula: C₂₃H₂₀N₂O₅

Molecular Weight: 404.421

Accurate Mass: 404.137223

Percentage Composition: C 68.31%; H 4.98%; N 6.93%; O 19.78%

Use/Importance: Used for diagnosis of pancreatic function (via 4-aminobenzoic acid elimination)

>>Variant: (S)-form

CAS Registry Number: 37106-97-1

Molecular Formula: C₂₃H₂₀N₂O₅

Molecular Weight: 404.421

Accurate Mass: 404.137223

Percentage Composition: C 68.31%; H 4.98%; N 6.93%; O 19.78%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 240-242°

Optical Rotation: [α]_D²⁵+72.3 (c, 0.03 in DMF)

Calculated Log P Data: Log P 2.96 (calc)

Hazard & Toxicity: LD₅₀ (rat, ipr) 2000 mg/kg

References:

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Bornschein, W. *et al.*, *Clin. Chim. Acta*, 1976, **67**, 21, (*use*)

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Martindale, The Extra Pharmacopoeia, 30th edn., Pharmaceutical Press, 1993, 773

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, CML835