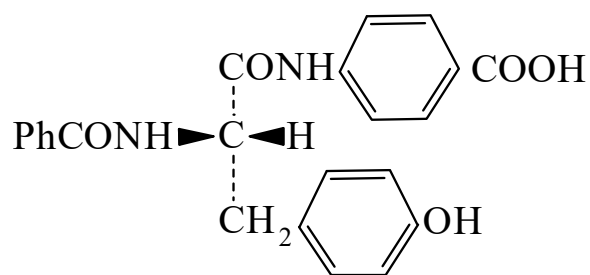




>>Entry Name: Bentiromide, BAN, INN, JAN, USAN

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: C<sub>23</sub>H<sub>20</sub>N<sub>2</sub>O<sub>5</sub>

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: C<sub>23</sub>H<sub>20</sub>N<sub>2</sub>O<sub>5</sub>

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]<sub>D</sub><sup>25</sup>+72.3 (c, 0.03 in DMF)

Calculated Log P Data: Log P 2.96 (calc)

Hazard & Toxicity: LD<sub>50</sub> (rat, ipr) 2000 mg/kg

#### References:

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Matsuda, M., *Pancreatic Function Diagnostants*, (Ed.), Igaku Shoin, Tokyo, 1980, (*book*)

*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