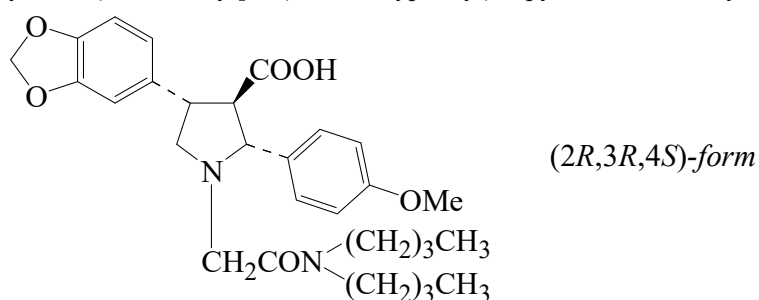




>>Entry Name: Atrasentan, INN

Synonym(s): 4-(1,3-Benzodioxol-5-yl)-1-[2-(dibutylamino)-2-oxoethyl]-2-(4-methoxyphenyl)-3-pyrrolidinecarboxylic acid, 9Cl. A 127722



CAS Registry Number: 195733-43-8

Molecular Formula: C₂₉H₃₈N₂O₆

Molecular Weight: 510.629

Accurate Mass: 510.272988

Percentage Composition: C 68.21%; H 7.50%; N 5.49%; O 18.80%

Biological Use/Importance: ET_A selective endothelin receptor antagonist. Antineoplastic agent for prostate cancer

>>Variant: (2R,3R,4S)-form

Synonym(s): ABT 627

CAS Registry Number: 173937-91-2

Molecular Formula: C₂₉H₃₈N₂O₆

Molecular Weight: 510.629

Accurate Mass: 510.272988

Percentage Composition: C 68.21%; H 7.50%; N 5.49%; O 18.80%

Other Data: Pharmacol. active isomer

>>Variant: (2RS,3RS,4SR)-form

Synonym(s): *trans,trans*-form

CAS Registry Number: 195704-72-4

Molecular Formula: C₂₉H₃₈N₂O₆

Molecular Weight: 510.629

Accurate Mass: 510.272988

Percentage Composition: C 68.21%; H 7.50%; N 5.49%; O 18.80%

Melting Point: Mp 122-124°

>>Variant: (2RS,3SR,4RS)-form

Synonym(s): *cis,trans*-form

Molecular Formula: C₂₉H₃₈N₂O₆

Molecular Weight: 510.629

Accurate Mass: 510.272988

Percentage Composition: C 68.21%; H 7.50%; N 5.49%; O 18.80%

Melting Point: Mp 165-166°

References:

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Jarvis, M.F. *et al.*, *Eur. J. Pharmacol.*, 2000, **388**, 29-35, (*pharmacol*)