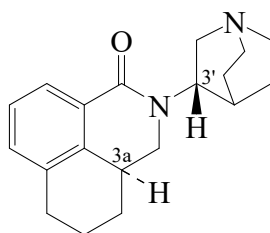




>>>Entry Name: Palonosetron, INN

Synonym(s): 2-(1-Azabicyclo[2.2.2]oct-3-yl)-2,3,3*a*,4,5,6-hexahydro-1*H*-benz[*d,e*]isoquinolin-1-one, 9Cl. 2,3,3*a*,4,5,6-Hexahydro-2-(3-quinuclidinyl)-1*H*-benz[*d,e*]isoquinolin-1-one. RS 25259-197



(3*aS*,3'*S*)-form

CAS Registry Number: 135729-60-1

Related CAS Registry Numbers(s): 135729-74-7 187033-23-4

Molecular Formula: C₁₉H₂₄N₂O

Molecular Weight: 296.411

Accurate Mass: 296.188863

Percentage Composition: C 76.99%; H 8.16%; N 9.45%; O 5.40%

Use/Importance: 5-HT₃-receptor antagonist. Antiemetic

Other Data: Palonosetron refers to the (3*aS*,3'*S*)-form

>>>Variant: (3*aR*,3'*R*)-form

CAS Registry Number: 149653-99-6

Molecular Formula: C₁₉H₂₄N₂O

Molecular Weight: 296.411

Accurate Mass: 296.188863

Percentage Composition: C 76.99%; H 8.16%; N 9.45%; O 5.40%

>>>Derivative: Hydrochloride

CAS Registry Number: 135729-75-8

Physical Description: Cryst. (EtOH/Et₂O)

Optical Rotation: $[\alpha]_{\text{D}}^{25} +94.7$ (c, 0.2 in H₂O)

Other Data: Mp >280°

>>>Variant: (3*aR*,3'*S*)-form

CAS Registry Number: 135729-73-6

Molecular Formula: C₁₉H₂₄N₂O

Molecular Weight: 296.411

Accurate Mass: 296.188863

Percentage Composition: C 76.99%; H 8.16%; N 9.45%; O 5.40%

>>>Derivative: Hydrochloride

CAS Registry Number: 135755-51-0

Physical Description: Cryst. (EtOH)

Melting Point: Mp 272-274°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +80$ (c, 0.2 in H₂O)

>>>Variant: (3*aS*,3'*R*)-form

CAS Registry Number: 149654-00-2

Molecular Formula: C₁₉H₂₄N₂O

Molecular Weight: 296.411

Accurate Mass: 296.188863

Percentage Composition: C 76.99%; H 8.16%; N 9.45%; O 5.40%

>>>Derivative: Hydrochloride

CAS Registry Number: 135729-76-9

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 275-276°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -67.6$ (c, 0.3 in H₂O)