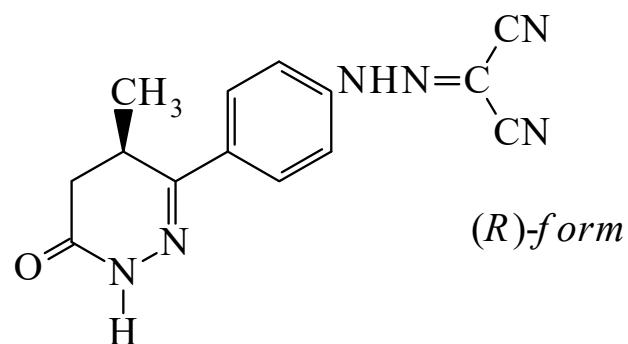




>>Entry Name: Simendan, INN

Synonym(s): [[4-(1,4,5,6-Tetrahydro-4-methyl-6-oxo-3-pyridazinyl)phenyl]hydrazaono]propanedinitrile, 9Cl



CAS Registry Number: 131741-08-7

Molecular Formula: C₁₄H₁₂N₆O

Molecular Weight: 280.288

Accurate Mass: 280.107259

Percentage Composition: C 59.99%; H 4.32%; N 29.98%; O 5.71%

Use/Importance: Cardiotonic agent. Phosphodiesterase (type III) inhibitor

>>Variant: (R)-form

Synonym(s): Levosimendan, INN. OR-1259

CAS Registry Number: 141505-33-1

Molecular Formula: C₁₄H₁₂N₆O

Molecular Weight: 280.288

Accurate Mass: 280.107259

Percentage Composition: C 59.99%; H 4.32%; N 29.98%; O 5.71%

Development Status: Phase III clinical trials (US, 1995)

Melting Point: Mp 210-214°

Optical Rotation: $[\alpha]_D^{25} -566$ (THF/MeOH)

Other Data: Pharmacol. active isomer

>>Variant: (S)-form

CAS Registry Number: 144238-75-5

Molecular Formula: C₁₄H₁₂N₆O

Molecular Weight: 280.288

Accurate Mass: 280.107259

Percentage Composition: C 59.99%; H 4.32%; N 29.98%; O 5.71%

Melting Point: Mp 210-214°

Optical Rotation: $[\alpha]_D^{25} +568$ (THF/MeOH)

>>Variant: (±)-form

CAS Registry Number: 157968-98-4

Molecular Formula: C₁₄H₁₂N₆O

Molecular Weight: 280.288

Accurate Mass: 280.107259

Percentage Composition: C 59.99%; H 4.32%; N 29.98%; O 5.71%

Melting Point: Mp 258-263°

References:

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