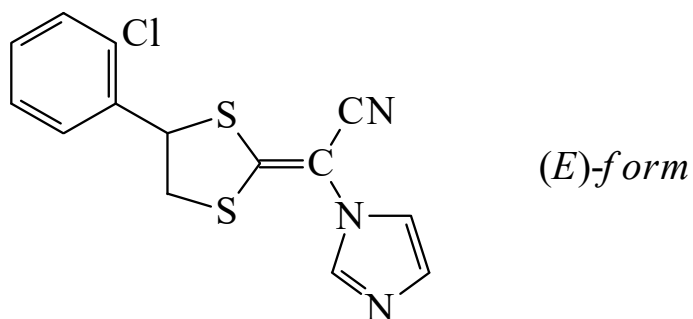




>>Entry Name: Lanoconazole, INN

Synonym(s): α -[4-(2-Chlorophenyl)-1,3-dithiolan-2-ylidene]-1*H*-imidazole-1-acetonitrile, 9Cl. Astat. NND 318



CAS Registry Number: 126509-69-1

Related CAS Registry Numbers(s): 133162-79-5 133162-80-8 133162-81-9 133267-38-6 153222-92-5 153222-93-6

Molecular Formula: C₁₄H₁₀ClN₃S₂

Molecular Weight: 319.838

Accurate Mass: 319.000464

Percentage Composition: C 52.57%; H 3.15%; Cl 11.08%; N 13.14%; S 20.05%

Use/Importance: Antifungal agent

Development Status: Launched 1994 (Japan)

Calculated Log P Data: Log P 2.87 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 652 mg/kg. LD₅₀ (rat, ipr) 1655 mg/kg. Exp. reprod. effects

>>Variant: (±)-(*E*)-form

CAS Registry Number: 101530-10-3

Molecular Formula: C₁₄H₁₀ClN₃S₂

Molecular Weight: 319.838

Accurate Mass: 319.000464

Percentage Composition: C 52.57%; H 3.15%; Cl 11.08%; N 13.14%; S 20.05%

Physical Description: Light yellow cryst.

Melting Point: Mp 141.5°

>>Variant: (±)-(*Z*)-form

CAS Registry Number: 101529-65-1

Molecular Formula: C₁₄H₁₀ClN₃S₂

Molecular Weight: 319.838

Accurate Mass: 319.000464

Percentage Composition: C 52.57%; H 3.15%; Cl 11.08%; N 13.14%; S 20.05%

Physical Description: Light yellow cryst.

Melting Point: Mp 119.4°

References:

Eur. Pat., 1987, *Nihon Nohyaku*, 218 736; *CA*, **107**, 134306r, (*synth*)

Japan. Pat., 1990, *Nihon Nohyaku*, 02 275 877; *CA*, **114**, 185474w, (*synth, isomers*)

Ohmi, T. *et al.*, *Arzneim.-Forsch.*, 1991, **41**, 847; 1992, **42**, 345, (*pharmacol*)

Niwano, Y. *et al.*, *Antimicrob. Agents Chemother.*, 1994, **38**, 2204, (*use*)