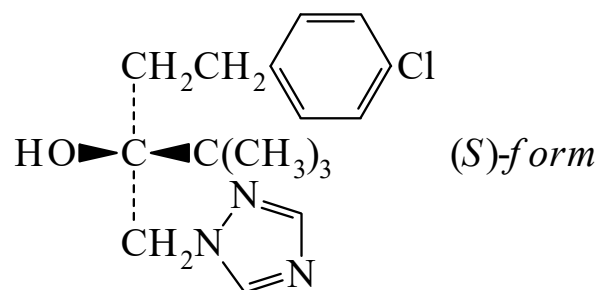




>>Entry Name: Tebuconazole, BSI

Synonym(s): α -[2-(4-Chlorophenyl)ethyl]- α -(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol, 9Cl. Folicur. Elite. Horizon. Lynx. Silvacur. Raxil. HWG-1608



CAS Registry Number: 80443-41-0

Related CAS Registry Numbers(s): 107534-96-3

Molecular Formula: C₁₆H₂₂ClN₃O

Molecular Weight: 307.822

Accurate Mass: 307.145139

Percentage Composition: C 62.43%; H 7.20%; Cl 11.52%; N 13.65%; O 5.20%

>>Variant: (*S*)-form

CAS Registry Number: 119364-85-1

Molecular Formula: C₁₆H₂₂ClN₃O

Molecular Weight: 307.822

Accurate Mass: 307.145139

Percentage Composition: C 62.43%; H 7.20%; Cl 11.52%; N 13.65%; O 5.20%

Use/Importance: Fungicide

Optical Rotation: $[\alpha]_{\text{D}}^{20} -34$ (c, 1 in CHCl₃)

Other Data: This is the more active enantiomer

>>Variant: ($\pm$)-form

CAS Registry Number: 107534-96-3

Molecular Formula: C₁₆H₂₂ClN₃O

Molecular Weight: 307.822

Accurate Mass: 307.145139

Percentage Composition: C 62.43%; H 7.20%; Cl 11.52%; N 13.65%; O 5.20%

Use/Importance: Fungicide. Steroid demethylation inhibitor

Physical Description: Cryst.

Melting Point: Mp 102.4°

Hazard & Toxicity: LD₅₀ (rat, orl) 4000 mg/kg

References:

Ger. Pat., 1981, 3 018 866; *CA*, **96**, 69004d, (*synth, activity*)

Kaspers, H. *et al.*, *Pflanzenschutz-Nachr.*, 1987, **40**, 81; 111; 133, (*synth, activity, props, tox*)

Kaulen, J., *Angew. Chem., Int. Ed.*, 1989, **28**, 462, (*synth, abs config, bibl*)

Pesticide Manual, 9th edn., 1991, No. 11185

Agrochemicals Handbook, 3rd edn., Royal Society of Chemistry, 1992, A1184