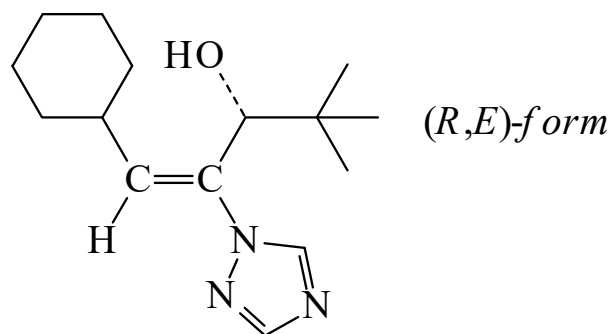




>>Entry Name: Triapenthenol, BSI

Synonym(s):  $\beta$ -(Cyclohexylmethylene)- $\alpha$ -(1,1-dimethylethyl)-1*H*-1,2,4-triazole-1-ethanol, 9Cl. 1-Cyclohexyl-4,4-dimethyl-2-(1*H*-1,2,4-triazol-1-yl)-1-penten-3-ol. Triapentenol. RSW 0411



CAS Registry Number: 76608-88-3

Related CAS Registry Numbers(s): 76608-49-6 76608-66-7 103238-73-9

Molecular Formula: C<sub>15</sub>H<sub>25</sub>N<sub>3</sub>O

Molecular Weight: 263.382

Accurate Mass: 263.199762

Percentage Composition: C 68.40%; H 9.57%; N 15.95%; O 6.07%

>>Variant: (*R,E*)-form

CAS Registry Number: 93851-05-9

Molecular Formula: C<sub>15</sub>H<sub>25</sub>N<sub>3</sub>O

Molecular Weight: 263.382

Accurate Mass: 263.199762

Percentage Composition: C 68.40%; H 9.57%; N 15.95%; O 6.07%

Use/Importance: Fungicide; inhibits steroid demethylation

Other Data: (+)ve opt. rotn.

>>Variant: (*S,E*)-form

CAS Registry Number: 93851-06-0

Molecular Formula: C<sub>15</sub>H<sub>25</sub>N<sub>3</sub>O

Molecular Weight: 263.382

Accurate Mass: 263.199762

Percentage Composition: C 68.40%; H 9.57%; N 15.95%; O 6.07%

Use/Importance: Plant growth regulator; inhibits gibberellin biosynth.

Other Data: (-)ve opt. rotn.

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

CAS Registry Number: 93851-03-7

Molecular Formula: C<sub>15</sub>H<sub>25</sub>N<sub>3</sub>O

Molecular Weight: 263.382

Accurate Mass: 263.199762

Percentage Composition: C 68.40%; H 9.57%; N 15.95%; O 6.07%

Use/Importance: Plant growth regulator. Gibberellin synth. inhibitor

Physical Description: Cryst.

Melting Point: Mp 135.5°

Hazard & Toxicity: LD<sub>50</sub> (rat, orl) >5000 mg/kg

#### References:

Ger. Pat., 1984, 3 302 120; CA, **102**, 24628m, (synth, resoln, activity, *R*-form)

Ger. Pat., 1984, 3 302 122; CA, **102**, 24629m, (synth, resoln, activity, *S*-form)

Luerssen, K. *et al.*, *Pestic. Sci.*, 1987, **19**, 153, (props)

Tombo, G.M.R. *et al.*, *Angew. Chem., Int. Ed.*, 1991, **30**, 1193, (rev)

*Pesticide Manual*, 9th edn., 1991, No. 11853