Acta Crystallographica Section E
**Structure Reports**
**Online**
ISSN 1600-5368

# 1-(4-Chlorophenyl)-4,4-dimethyl-3-(4*H*-1,2,4-triazol-4-ylmethyl)pentan-3-ol monohydrate

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Received 10 April 2006
Accepted 27 April 2006

**Key indicators**

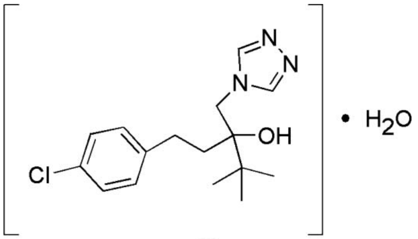
Single-crystal X-ray study
*T* = 295 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.056
*wR* factor = 0.180
Data-to-parameter ratio = 17.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{16}H_{22}ClN_3O\cdot H_2O$, was obtained as a by-product during the attempted preparation of tebuconazole. In the molecule, the triazole ring is approximately perpendicular to the benzene ring. The crystal structure is consolidated by O—H···O and O—H···N intermolecular hydrogen bonding.

## Comment

Tebuconazole [systematic name: 1-(4-chlorophenyl)-4,4-dimethyl-3-(1*H*-1,2,4-triazol-1-ylmethyl)pentan-3-ol] is an effective triazole fungicide against various types of smut and numerous pathogens, which is widely used for seed dressing and spraying crops. Its isomer, 1-(4-chlorophenyl)-4,4-dimethyl-3-(4*H*-1,2,4-triazol-4-yl-methyl)-pentan-3-ol monohydrate, (I), was obtained as a by-product during the attempted preparation of tebuconazole.



**(I)**

The molecular structure of (I) is shown in Fig. 1. The molecule contains a planar 1,2,4-triazole ring and a benzene ring. The triazole ring is approximately perpendicular to the benzene ring with a dihedral angle of 88.9 (2)°.

The uncoordinated water molecule links with the triazole ring *via* O—H···N hydrogen bonding (Table 1). The combi-

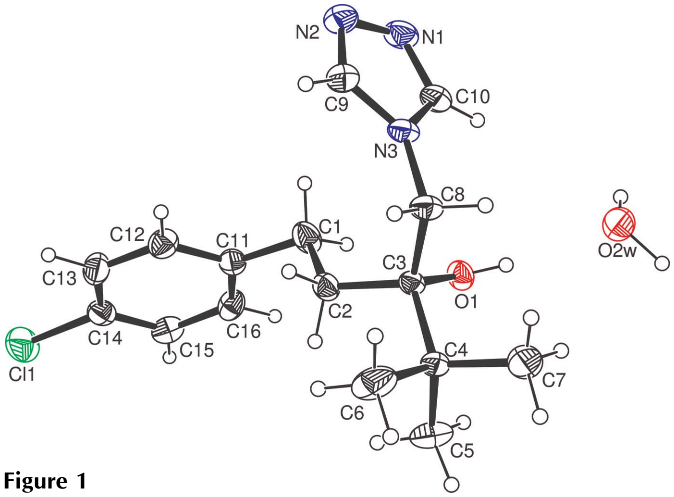


**Figure 1**
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

doi:10.1107/S1600536806015376

nation of four O—H···N hydrogen bonds generates a centrosymmetric $R_4^4(10)$ aggregate of six molecules (Bernstein *et al.*, 1995) (Fig. 2). The hydroxy group is also hydrogen bonded with the uncoordinated water molecule.

## Experimental

1-*tert*-Butyl-1-(4-chlorophenylethyl)oxirane (120 g) was added to an *n*-butanol solution (100 ml) of KOH (3 g) and 1,2,4-triazole (40 g). The mixture was refluxed for 6 h and then neutralized with an aqueous solution of HCl (Raya *et al.*, 2003). The organic layer was separated from the mixture and cooled in an ice bath, giving a white precipitate. It was dissolved in cyclohexane (500 ml) and crystals of (I) grew from the solution in a low yield (5 g). Single crystals of (I) were obtained by recrystallization of an ethanol/ethyl acetate solution (1:5 *v*/*v*).

### Crystal data

$C_{16}H_{22}ClN_3O \cdot H_2O$
$M_r = 325.83$
Triclinic, $P\bar{1}$
$a = 7.6326$ (5) Å
$b = 8.6811$ (6) Å
$c = 13.0126$ (9) Å
$\alpha = 84.223$ (1)°
$\beta = 86.284$ (1)°
$\gamma = 80.483$ (1)°
$V = 845.0$ (1) Å$^3$
$Z = 2$
$D_x = 1.281$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.24$ mm$^{-1}$
$T = 295$ (2) K
Block, colorless
0.44 × 0.37 × 0.21 mm

### Data collection

Bruker AXS SMART 1000 CCD diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.903$, $T_{max} = 0.952$
6924 measured reflections
3587 independent reflections
2291 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.1°$

### Refinement

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.180$
$S = 1.09$
3587 reflections
211 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0831P)^2 + 0.071P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.75$ e Å$^{-3}$
$\Delta\rho_{min} = -0.45$ e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O2*W* | 0.82 | 2.02 | 2.830 (3) | 168 |
| O2*W*—H2*C*···N1$^{i}$ | 0.79 (4) | 2.11 (4) | 2.888 (3) | 166 (3) |
| O2*W*—H2*D*···N2$^{ii}$ | 0.97 (4) | 2.00 (4) | 2.951 (3) | 166 (3) |

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $x, y-1, z$.

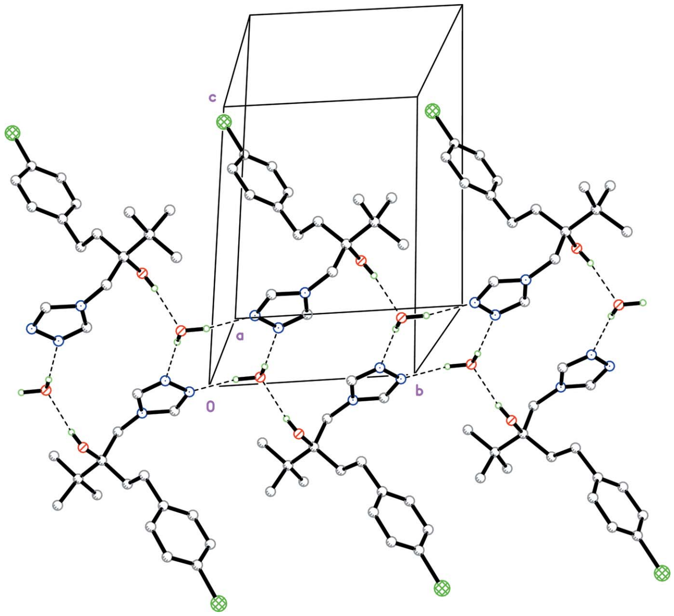


**Figure 2**
A packing diagram for (I). H atoms bonded to C atoms have been omitted for clarity. Dashed lines indicate hydrogen bonds.

The hydroxy H atom was positioned geometrically (O—H = 0.82 Å) and refined as riding [$U_{iso}(H) = 1.5U_{eq}(O)$]. H atoms of the water molecule were located in a difference Fourier map and refined isotropically. Methyl H atoms were positioned geometrically (C—H = 0.96 Å) and torsion angles refined to fit the electron density [$U_{iso}(H) = 1.5U_{eq}(C)$]. Other H atoms were placed in calculated positions (methylene C—H = 0.97 Å and aromatic C—H = 0.93 Å) and refined as riding [$U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 1997).

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