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1-{[1-(2,4-Dichlorophenyl)-1,3-dioxolan-2-yl]-methyl}-1*H*-1,2,4-triazole

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In the title compound, $C_{12}H_{11}Cl_2N_3O_2$, also referred to as azaconazole, the five-membered 1,3-dioxolane ring assumes an envelope conformation. In the crystal packing, the molecules are linked into an extended three-dimensional network by weak C—H···O interactions.

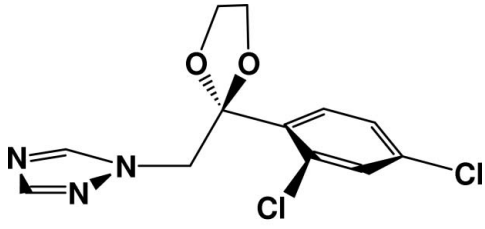
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.057
wR factor = 0.102
Data-to-parameter ratio = 14.9

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

Comment

The title compound, (I), also referred to as azaconazole, is a well known agricultural fungicide and wood preservative (Van Gestel *et al.*, 1980; Van Leemput, Swysen *et al.*, 1987; Heeres, 1984). Compound (I) was also used as a technical aid in mushroom cultivation (Van Leemput, Demoen, *et al.*, 1987). A search of the Cambridge Structural Database (CSD, Version 5.27; Allen, 2002) revealed that no crystallographic data are available for (I). Therefore, a single-crystal structural analysis of (I) was carried out in order to elucidate its structure and the results are reported here.



(I)

In the molecule of (I), bond distances and angles are within the expected ranges (Allen *et al.*, 1987). The 1,3-dioxolane ring (O1/O2/C4–C6) adopts an envelope conformation, with puckering parameters Q_2 = 0.281 (2) Å and φ_2 = 34.8 (6)° (Cremer & Pople, 1975). The triazole ring (N1–N3/C1/C2) is essentially planar [maximum displacement 0.054 (4) Å for atom C1] and forms a dihedral angle of 20.32 (9)° with the benzene ring (C7–C12).

The crystal packing of (I) is stabilized by weak intra- and intermolecular C—H···O hydrogen-bond interactions (Table 1, Fig. 2).

Experimental

The title compound was synthesized according to the literature method of Yang *et al.* (2001). Colourless single crystals of (I) were obtained by slow evaporation of an ethanol solution at 298 K. Elemental analysis, calculated for $C_{12}H_{11}Cl_2N_3O_2$: C 48.02, H 3.66, N 14.01%; found: C 47.95, H 3.66, N 13.98%.

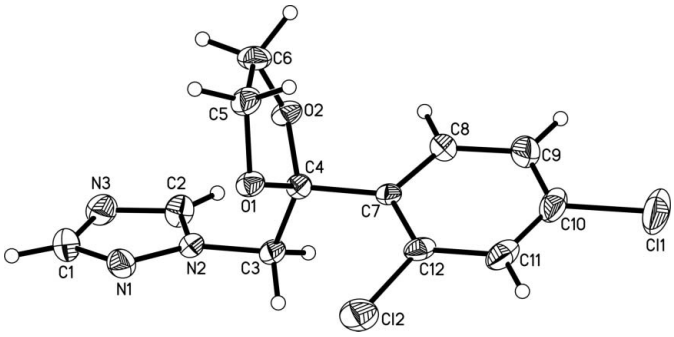


Figure 1
The structure of (I), with 30% probability displacement ellipsoids.

Crystal data

$C_{12}H_{11}Cl_2N_3O_2$
M_r = 300.14
Orthorhombic, *Pbca*
a = 11.121 (2) Å
b = 7.2420 (14) Å
c = 32.691 (7) Å
V = 2632.9 (9) Å^3
Z = 8
D_x = 1.514 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 298 (2) K
Block, colourless
0.40 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.827, T_{max} = 0.952
5108 measured reflections
2584 independent reflections
1580 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 26.0°
3 standard reflections
every 97 reflections
intensity decay: 8.4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.102
S = 1.03
2584 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 0.55P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0032 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O2	0.93	2.31	2.689 (3)	104
C3—H3A···O2^{i}	0.97	2.35	3.306 (4)	168

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z$.

All H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

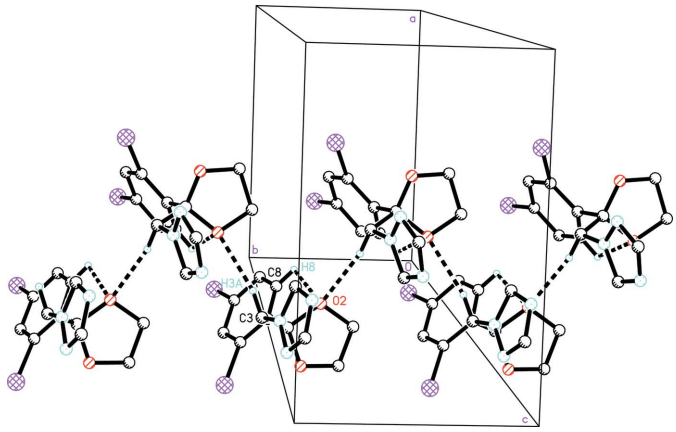


Figure 2
A partial packing diagram for the title compound, showing the C—H···O hydrogen-bond interactions (dashed lines).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1998); software used to prepare material for publication: *SHELXL97*.

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