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1-(4-Chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl)-2-butyl chloroacetate

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In the title compound, $C_{16}H_{19}Cl_2N_3O_2$, the dihedral angle between the two rings is 86.26 (2)°. The crystal packing is stabilized mainly by van der Waals interactions.

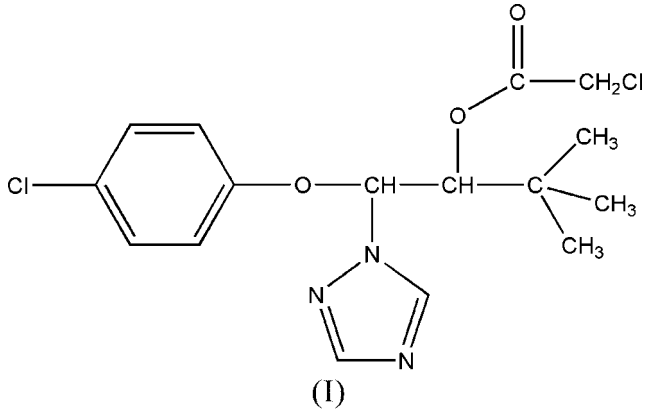
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.075
Data-to-parameter ratio = 16.6

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

Comment

Triadimenol is a commercial fungicide with some interesting features. Based on triadimenol, many modified derivatives have been synthesized in order to search for new highly fungicidal triazole compounds, including the title compound, (I) (Kraemer, 1976). Here, we describe the crystal structure of compound (I).



(I)

The bond lengths and angles in (I) (Table 1) are in agreement with the values quoted in previous reports of the related compounds 1-(4-hydroxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one (Xu *et al.*, 2004) and 1-(4-chlorophenyl)-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one (Liu *et al.*, 2005). The dihedral angle between the two ring planes is 86.26 (2)°.

Experimental

A mixture of triadimenol (2.95 g, 0.01 mol), potassium carbonate (1.38 g, 0.01 mol) and chloroacetyl chloride (1.13 g, 0.01 mol) was refluxed in dichloromethane (10 ml) for 5 h to afford the title compound (yield 1.85 g, 50%). Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from acetone at room temperature.

Crystal data

$C_{16}H_{19}Cl_2N_3O_3$
M_r = 372.24
Orthorhombic, $P2_12_12_1$
a = 10.1456 (15) Å
b = 10.7610 (17) Å
c = 16.481 (3) Å
V = 1799.3 (5) Å^3
Z = 4
D_x = 1.374 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 294 (2) K
Block, colourless
0.24 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.914, T_{max} = 0.963
10202 measured reflections
3673 independent reflections
2765 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.075
S = 1.04
3673 reflections
221 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0286P)^2 + 0.1498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), with 1568 Friedel pairs
Flack parameter: 0.28 (6)

Table 1
Selected geometric parameters (Å, °).

Cl1—C4	1.753 (2)	N1—N2	1.353 (2)
Cl2—C16	1.765 (3)	N1—C7	1.467 (3)
O1—C1	1.386 (2)	C8—N3	1.319 (3)
O1—C7	1.411 (2)	C9—N2	1.318 (3)
O2—C15	1.342 (3)		
C1—O1—C7	118.36 (16)	O1—C7—C10	109.79 (17)
C2—C1—O1	124.89 (19)	N1—C7—C10	111.00 (17)
O1—C1—C6	114.83 (19)	O2—C10—C7	108.22 (17)
O1—C7—N1	108.53 (17)	O2—C10—C11	108.35 (17)

All H atoms were placed in calculated positions, with C—H = 0.93–0.98 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) for the aryl and methylene H atoms and 1.5U_{eq}(C) for the methyl H atoms. The value of the Flack parameter suggests partial inversion twinning.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

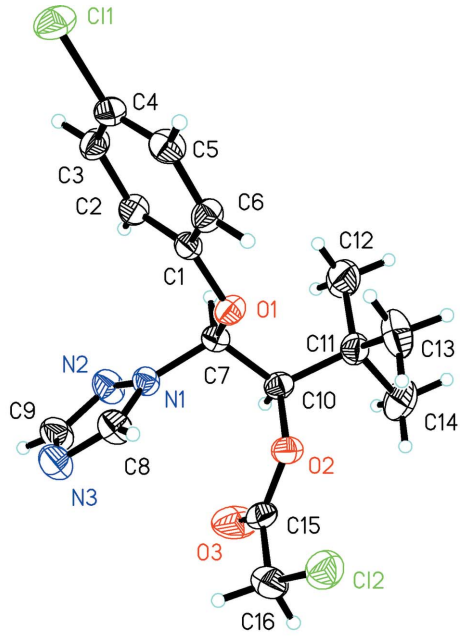


Figure 1
The molecular structure of compound (I), with displacement ellipsoids drawn at the 40% probability level.

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