

Imazalil: 1-[2-(2,4-dichlorophenyl)-2-(prop-2-enyloxy)ethyl]-1*H*-imidazole

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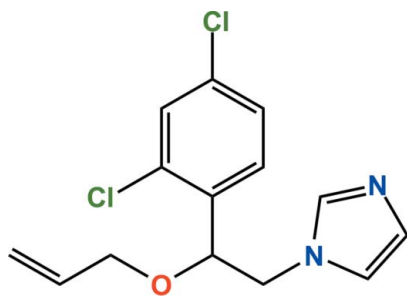
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.046; wR factor = 0.119; data-to-parameter ratio = 17.7.

In the title compound, $\text{C}_{14}\text{H}_{14}\text{Cl}_2\text{N}_2\text{O}$, the imidazole ring is almost parallel to the benzene ring, the dihedral angle between them being $7.3(2)^\circ$. In the crystal, there is an intermolecular $\text{C}-\text{Cl}\cdots\pi$ interaction ($\text{Cl}\cdots\text{centroid} = 3.36$ Å and $\text{C}-\text{Cl}\cdots\text{centroid} = 89.2^\circ$). In addition, a $\text{Cl}\cdots\text{Cl}$ contact of $3.411(1)$ Å and an intermolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bond are observed. These interactions contribute to the stabilization of the crystal packing.

Related literature

For information on the toxicity of the title compound, see: Sisman & Türkez (2010). For related structures, see: Bisaha *et al.* (2005).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{14}\text{Cl}_2\text{N}_2\text{O}$
 $M_r = 297.17$
 Monoclinic, $P2_1/c$
 $a = 7.9374(6)$ Å
 $b = 13.4144(12)$ Å
 $c = 13.479(1)$ Å
 $\beta = 103.386(5)^\circ$
 $V = 1396.19(19)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.46$ mm⁻¹
 $T = 173$ K
 $0.20 \times 0.09 \times 0.08$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.914$, $T_{\max} = 0.964$
 12201 measured reflections
 3040 independent reflections
 2282 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.069$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.119$
 $S = 1.08$
 3040 reflections
 172 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.37$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.27$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4}-\text{H4}\cdots\text{N2}^i$	0.95	2.66	3.562 (3)	159

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

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2006); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL and DIAMOND (Brandenburg, 1998); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2433).

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supplementary materials

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Imazalil: 1-[2-(2,4-dichlorophenyl)-2-(prop-2-enyloxy)ethyl]-1*H*-imidazole

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Comment

Imazalil (systematic name: 1-[2-(2,4-dichlorophenyl)-2-(2-propen-1-yloxy)ethyl]-1*H*-imidazole) is a fungicide widely used in agriculture, particularly in the growth of citrus fruits. It is also known as "enilconazole" (Sisman & Türkez, 2010). However, until now its crystal structure has not been reported.

In the title compound (Fig. 1), the imidazole ring is almost parallel to the benzene ring, the dihedral angle between them being 7.3 (2)°. All bond lengths and bond angles are normal and comparable to those observed in similar crystal structures (Bisaha *et al.* 2005).

In the crystal structure, as shown in Fig. 2, weak intermolecular C—H···N hydrogen bonds (Table 1) and a Cl···Cl contact of 3.411 (1) Å are observed. There are also C—Cl··· π interactions involving chlorine Cl2 and benzene ring (C1–C6), with a Cl···centroid (Cg^{iii}) distance of 3.36 Å and a C3—Cl2··· Cg^{iii} angle of 89.2° [symmetry code: (iii) $-x + 1, -y + 2, -z + 1$] (Fig. 2). These intermolecular interactions may contribute to the stabilization of the crystal packing.

Experimental

The title compound was purchased from the Dr. Ehrenstorfer GmbH Company. Slow evaporation of a solution in CH₂Cl₂ gave single crystals suitable for X-ray analysis.

Refinement

The H atoms were geometrically positioned and refined as riding. C—H = 0.95 Å for Csp², C—H = 0.99 Å for methylene C and C—H = 1.00 Å for methine C; $U_{iso}(H) = 1.2U_{eq}(\text{parent atom})$.

Figures

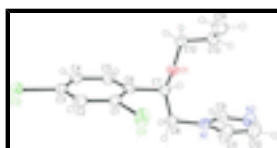


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

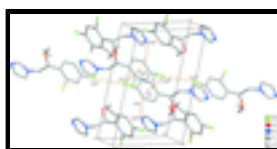


Fig. 2. Crystal packing of the title compound with intermolecular C—H···N hydrogen bonds, C—Cl··· π interactions and Cl···Cl contacts shown as dashed lines. H atoms not involved in intermolecular interactions have been omitted for clarity. [Symmetry codes: (i) $-x + 2, -y + 2, -z + 1$; (ii) $x + 1, -y + 1.5, z + 1/2$; (iii) $-x + 1, -y + 2, -z + 1$; (iv) $-x, y + 1/2, -z + 1/2$; (v) $x - 1, y, z$.]

1-[2-(2,4-dichlorophenyl)-2-(prop-2-enyloxy)ethyl]-1*H*-imidazole

Crystal data

$C_{14}H_{14}Cl_2N_2O$	$F(000) = 616$
$M_r = 297.17$	$D_x = 1.414 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ybc	Cell parameters from 2420 reflections
$a = 7.9374 (6) \text{ \AA}$	$\theta = 2.2\text{--}28.4^\circ$
$b = 13.4144 (12) \text{ \AA}$	$\mu = 0.46 \text{ mm}^{-1}$
$c = 13.479 (1) \text{ \AA}$	$T = 173 \text{ K}$
$\beta = 103.386 (5)^\circ$	Plate, colourless
$V = 1396.19 (19) \text{ \AA}^3$	$0.20 \times 0.09 \times 0.08 \text{ mm}$
$Z = 4$	

Data collection

Bruker APEXII CCD diffractometer	3040 independent reflections
Radiation source: fine-focus sealed tube graphite	2282 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.069$
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	$\theta_{\text{max}} = 27.0^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.914$, $T_{\text{max}} = 0.964$	$h = -9 \rightarrow 10$
12201 measured reflections	$k = -17 \rightarrow 14$
	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.119$	H-atom parameters constrained
$S = 1.08$	$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.2498P]$
3040 reflections	where $P = (F_o^2 + 2F_c^2)/3$
172 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.37 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.41595 (8)	0.69956 (5)	0.57733 (5)	0.0410 (2)
C12	0.77994 (7)	0.98990 (4)	0.47431 (5)	0.03569 (19)
O1	0.0431 (2)	0.71310 (11)	0.25901 (12)	0.0294 (4)
N1	-0.1440 (2)	0.69576 (14)	0.40437 (15)	0.0289 (4)
N2	-0.3936 (3)	0.60867 (17)	0.34432 (19)	0.0465 (6)
C1	0.4327 (3)	0.78309 (16)	0.48568 (17)	0.0282 (5)
C2	0.5822 (3)	0.84344 (16)	0.51200 (18)	0.0285 (5)
H2	0.6668	0.8363	0.5742	0.034*
C3	0.5937 (3)	0.91175 (16)	0.44116 (18)	0.0279 (5)
C4	0.4636 (3)	0.91953 (16)	0.34627 (18)	0.0297 (5)
H4	0.4775	0.9689	0.2982	0.036*
C5	0.3172 (3)	0.85669 (16)	0.32241 (18)	0.0277 (5)
H5	0.2343	0.8632	0.2594	0.033*
C6	0.2977 (3)	0.78727 (15)	0.39102 (17)	0.0255 (5)
C7	0.1325 (3)	0.72205 (16)	0.36550 (17)	0.0253 (5)
H7	0.1605	0.6540	0.3949	0.030*
C8	-0.0025 (3)	0.76633 (17)	0.40885 (19)	0.0311 (5)
H8A	0.0469	0.7854	0.4806	0.037*
H8B	-0.0474	0.8274	0.3704	0.037*
C9	-0.3009 (3)	0.68361 (19)	0.3287 (2)	0.0377 (6)
H9	-0.3345	0.7269	0.2718	0.045*
C10	-0.2883 (4)	0.5710 (2)	0.4355 (2)	0.0505 (7)
H10	-0.3197	0.5139	0.4688	0.061*
C11	-0.1353 (4)	0.6230 (2)	0.4733 (2)	0.0440 (6)
H11	-0.0471	0.6102	0.5328	0.053*
C12	0.1149 (3)	0.63442 (17)	0.21546 (18)	0.0312 (5)
H12A	0.2426	0.6410	0.2344	0.037*
H12B	0.0777	0.6401	0.1403	0.037*
C13	0.0682 (3)	0.53464 (18)	0.24568 (19)	0.0350 (6)
H13	-0.0508	0.5167	0.2311	0.042*
C14	0.1862 (4)	0.4672 (2)	0.2933 (2)	0.0451 (7)
H14B	0.3060	0.4833	0.3087	0.054*
H14A	0.1493	0.4037	0.3112	0.054*

Atomic displacement parameters (\AA^2)

U^{11} U^{22} U^{33} U^{12} U^{13} U^{23}

supplementary materials

Cl1	0.0519 (4)	0.0404 (4)	0.0294 (3)	-0.0131 (3)	0.0066 (3)	0.0096 (3)
Cl2	0.0339 (3)	0.0338 (3)	0.0442 (4)	-0.0075 (2)	0.0189 (3)	-0.0031 (3)
O1	0.0340 (8)	0.0319 (8)	0.0244 (8)	0.0010 (7)	0.0111 (7)	-0.0023 (7)
N1	0.0320 (10)	0.0296 (10)	0.0285 (10)	0.0003 (8)	0.0139 (9)	-0.0005 (8)
N2	0.0390 (12)	0.0524 (14)	0.0515 (15)	-0.0104 (11)	0.0170 (11)	-0.0142 (12)
C1	0.0376 (12)	0.0253 (11)	0.0253 (12)	0.0009 (10)	0.0147 (10)	0.0020 (9)
C2	0.0310 (12)	0.0305 (12)	0.0256 (12)	0.0001 (10)	0.0098 (10)	-0.0012 (10)
C3	0.0286 (11)	0.0249 (11)	0.0347 (13)	-0.0021 (9)	0.0168 (10)	-0.0065 (10)
C4	0.0362 (12)	0.0251 (11)	0.0337 (13)	0.0022 (9)	0.0203 (11)	0.0035 (10)
C5	0.0305 (12)	0.0288 (12)	0.0256 (12)	0.0033 (9)	0.0104 (10)	0.0002 (10)
C6	0.0315 (12)	0.0233 (11)	0.0253 (11)	0.0030 (9)	0.0142 (10)	-0.0022 (9)
C7	0.0313 (11)	0.0236 (11)	0.0225 (11)	-0.0007 (9)	0.0090 (10)	-0.0019 (9)
C8	0.0399 (13)	0.0259 (12)	0.0324 (13)	-0.0017 (10)	0.0183 (11)	-0.0032 (10)
C9	0.0362 (13)	0.0440 (14)	0.0357 (14)	0.0031 (11)	0.0136 (12)	-0.0004 (12)
C10	0.0503 (16)	0.0398 (15)	0.066 (2)	-0.0085 (13)	0.0237 (16)	0.0085 (14)
C11	0.0441 (15)	0.0475 (15)	0.0410 (15)	-0.0023 (12)	0.0109 (13)	0.0163 (13)
C12	0.0367 (13)	0.0334 (12)	0.0277 (12)	-0.0062 (10)	0.0159 (11)	-0.0058 (10)
C13	0.0403 (13)	0.0357 (13)	0.0319 (13)	-0.0111 (11)	0.0143 (11)	-0.0077 (11)
C14	0.0631 (18)	0.0383 (14)	0.0387 (15)	-0.0040 (13)	0.0219 (14)	-0.0038 (12)

Geometric parameters (\AA , $^\circ$)

Cl1—C1	1.696 (2)	C5—H5	0.9500
Cl2—C3	1.783 (2)	C6—C7	1.547 (3)
O1—C12	1.392 (3)	C7—C8	1.461 (3)
O1—C7	1.452 (3)	C7—H7	1.0000
N1—C11	1.338 (3)	C8—H8A	0.9900
N1—C9	1.425 (3)	C8—H8B	0.9900
N1—C8	1.459 (3)	C9—H9	0.9500
N2—C9	1.291 (3)	C10—C11	1.391 (4)
N2—C10	1.410 (4)	C10—H10	0.9500
C1—C2	1.412 (3)	C11—H11	0.9500
C1—C6	1.465 (3)	C12—C13	1.471 (3)
C2—C3	1.342 (3)	C12—H12A	0.9900
C2—H2	0.9500	C12—H12B	0.9900
C3—C4	1.450 (3)	C13—C14	1.353 (4)
C4—C5	1.411 (3)	C13—H13	0.9500
C4—H4	0.9500	C14—H14B	0.9500
C5—C6	1.346 (3)	C14—H14A	0.9500
C12—O1—C7	108.98 (17)	C6—C7—H7	109.2
C11—N1—C9	108.0 (2)	N1—C8—C7	110.39 (18)
C11—N1—C8	121.9 (2)	N1—C8—H8A	109.6
C9—N1—C8	129.8 (2)	C7—C8—H8A	109.6
C9—N2—C10	100.1 (2)	N1—C8—H8B	109.6
C2—C1—C6	126.8 (2)	C7—C8—H8B	109.6
C2—C1—C11	113.51 (18)	H8A—C8—H8B	108.1
C6—C1—C11	119.65 (16)	N2—C9—N1	114.1 (2)
C3—C2—C1	113.9 (2)	N2—C9—H9	122.9
C3—C2—H2	123.1	N1—C9—H9	122.9

C1—C2—H2	123.1	C11—C10—N2	115.5 (2)
C2—C3—C4	121.7 (2)	C11—C10—H10	122.2
C2—C3—C12	114.37 (18)	N2—C10—H10	122.2
C4—C3—C12	123.96 (17)	N1—C11—C10	102.2 (2)
C5—C4—C3	122.6 (2)	N1—C11—H11	128.9
C5—C4—H4	118.7	C10—C11—H11	128.9
C3—C4—H4	118.7	O1—C12—C13	114.76 (18)
C6—C5—C4	118.4 (2)	O1—C12—H12A	108.6
C6—C5—H5	120.8	C13—C12—H12A	108.6
C4—C5—H5	120.8	O1—C12—H12B	108.6
C5—C6—C1	116.6 (2)	C13—C12—H12B	108.6
C5—C6—C7	117.7 (2)	H12A—C12—H12B	107.6
C1—C6—C7	125.69 (19)	C14—C13—C12	123.3 (2)
O1—C7—C8	101.13 (18)	C14—C13—H13	118.4
O1—C7—C6	117.51 (17)	C12—C13—H13	118.4
C8—C7—C6	110.10 (17)	C13—C14—H14B	120.0
O1—C7—H7	109.2	C13—C14—H14A	120.0
C8—C7—H7	109.2	H14B—C14—H14A	120.0
C6—C1—C2—C3	1.4 (3)	C1—C6—C7—O1	-160.79 (18)
C11—C1—C2—C3	-178.10 (16)	C5—C6—C7—C8	-93.1 (2)
C1—C2—C3—C4	-1.0 (3)	C1—C6—C7—C8	84.2 (3)
C1—C2—C3—C12	179.00 (15)	C11—N1—C8—C7	80.7 (3)
C2—C3—C4—C5	0.3 (3)	C9—N1—C8—C7	-93.6 (3)
C12—C3—C4—C5	-179.78 (16)	O1—C7—C8—N1	67.1 (2)
C3—C4—C5—C6	0.4 (3)	C6—C7—C8—N1	-167.88 (18)
C4—C5—C6—C1	-0.1 (3)	C10—N2—C9—N1	-0.1 (3)
C4—C5—C6—C7	177.48 (18)	C11—N1—C9—N2	0.2 (3)
C2—C1—C6—C5	-0.8 (3)	C8—N1—C9—N2	175.2 (2)
C11—C1—C6—C5	178.64 (16)	C9—N2—C10—C11	0.0 (3)
C2—C1—C6—C7	-178.2 (2)	C9—N1—C11—C10	-0.2 (3)
C11—C1—C6—C7	1.3 (3)	C8—N1—C11—C10	-175.6 (2)
C12—O1—C7—C8	-152.67 (17)	N2—C10—C11—N1	0.2 (3)
C12—O1—C7—C6	87.5 (2)	C7—O1—C12—C13	73.9 (2)
C5—C6—C7—O1	21.8 (3)	O1—C12—C13—C14	-120.4 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C4—H4...N2 ⁱ	0.95	2.66	3.562 (3)	159

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

Fig. 1

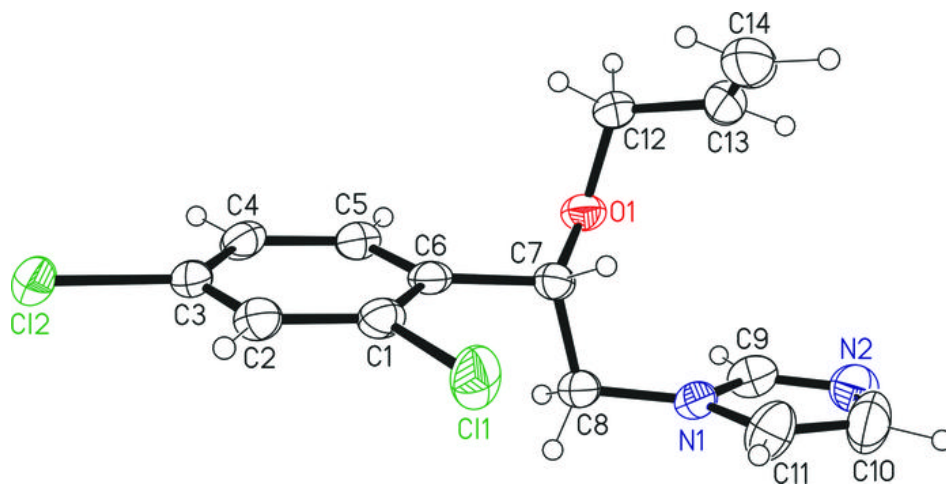


Fig. 2

