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

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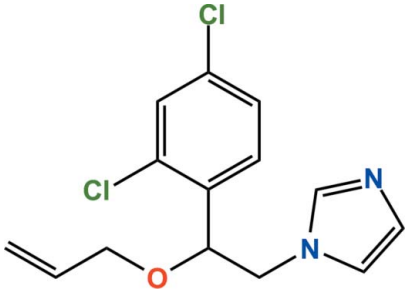
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.119; data-to-parameter ratio = 17.7.

In the title compound, $C_{14}H_{14}Cl_2N_2O$, the imidazole ring is almost parallel to the benzene ring, the dihedral angle between them being 7.3 (2)°. In the crystal, there is an intermolecular C—Cl···π interaction (Cl···centroid = 3.36 Å and C—Cl···centroid = 89.2°). In addition, a Cl···Cl contact of 3.411 (1) Å and an intermolecular C—H···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

$C_{14}H_{14}Cl_2N_2O$
M_r = 297.17
Monoclinic, $P2_1/c$
a = 7.9374 (6) Å
b = 13.4144 (12) Å
c = 13.479 (1) Å
β = 103.386 (5)°
V = 1396.19 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 173 K
0.20 × 0.09 × 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_{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
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···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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supporting information

Acta Cryst. (2011). E**67**, o1459 [doi:10.1107/S1600536811018241]

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

Sanghun Cheon, Yong Woon Shin, Ki-Min Park, Jineun Kim and Tae Ho Kim

S1. 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.

S2. Experimental

The title compound was purchased from the Dr. Ehrenstorfer GmbH Company. Slow evaporation of a solution in CH_2Cl_2 gave single crystals suitable for X-ray analysis.

S3. Refinement

The H atoms were geometrically positioned and refined as riding. C—H = 0.95 Å for Csp^2, C—H = 0.99 Å for methylene C and C—H = 1.00 Å for methine C; U_{iso}(H) = 1.2U_{eq}(parent atom).

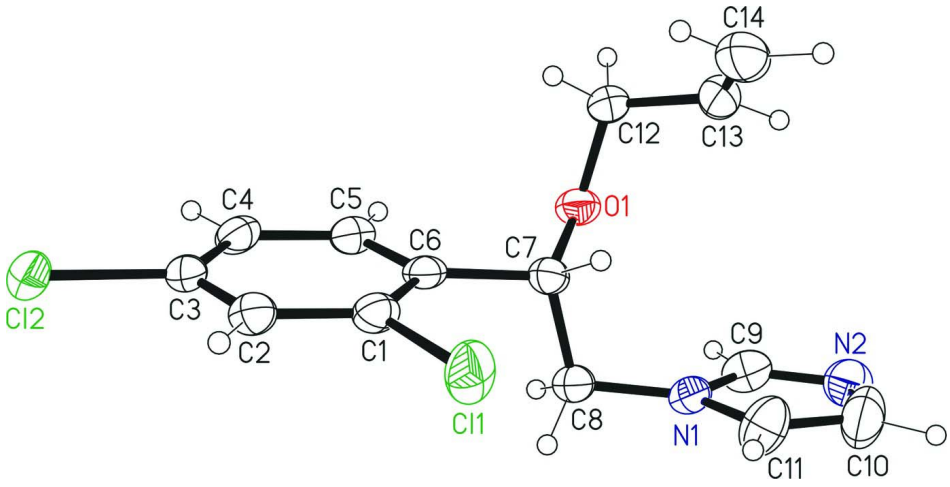

Figure 1

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.

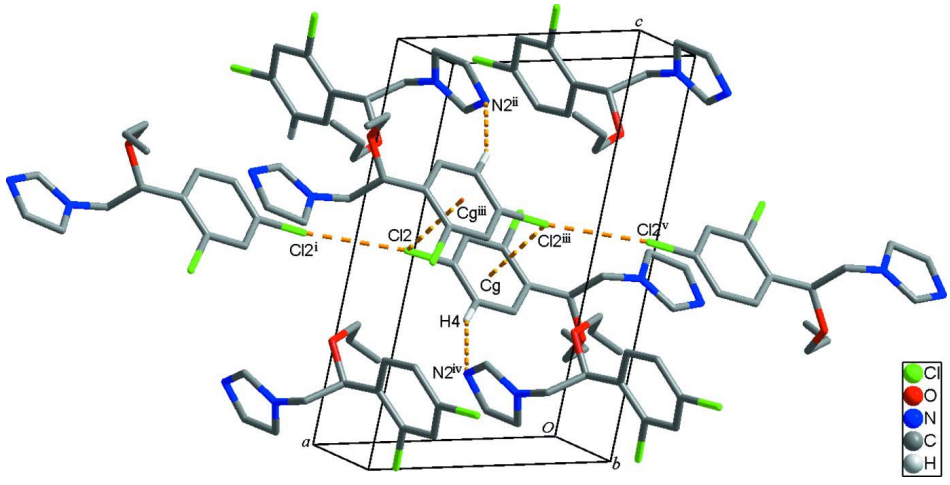

Figure 2

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

$C_{14}H_{14}Cl_2N_2O$
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c = 13.479 (1) Å
β = 103.386 (5)°
V = 1396.19 (19) Å^3
Z = 4
F(000) = 616
D_x = 1.414 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2420 reflections
θ = 2.2–28.4°
μ = 0.46 mm^{-1}

T = 173 K
Plate, colourless

0.20 × 0.09 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
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_{int} = 0.069
θ_{max} = 27.0°, θ_{min} = 2.2°
h = −9→10
k = −17→14
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.119
S = 1.08
3040 reflections
172 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.2498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.41595 (8)	0.69956 (5)	0.57733 (5)	0.0410 (2)
Cl2	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 (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
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 (Å, º)

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—Cl1	113.51 (18)	H8A—C8—H8B	108.1
C6—C1—Cl1	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—Cl2	114.37 (18)	N2—C10—H10	122.2
C4—C3—Cl2	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)
Cl1—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—Cl2	179.00 (15)	C11—N1—C8—C7	80.7 (3)

C2—C3—C4—C5	0.3 (3)	C9—N1—C8—C7	−93.6 (3)
Cl2—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)
Cl1—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)
Cl1—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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···N2^{i}	0.95	2.66	3.562 (3)	159

Symmetry code: (i) −*x*, *y*+1/2, −*z*+1/2.