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2-(2,4-Dichlorophenyl)-1*H*-benzimidazole

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.050
wR factor = 0.156
Data-to-parameter ratio = 16.8

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

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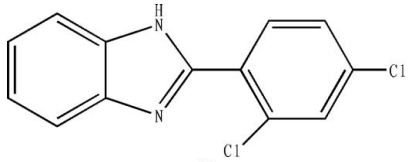
The title compound, $C_{13}H_8Cl_2N_2$, was prepared by reaction of *o*-phenylenediamine with 2,4-dichlorobenzaldehyde under reflux in ethanol. The dihedral angle between the benzimidazole system and the benzene ring is 42.00 (15)°. In the crystal structure, intermolecular N—H···N interactions are present.

Comment

There is growing interest in benzimidazole and its derivatives for their photoluminescent properties (Tong *et al.*, 2005; Wu *et al.*, 2003; Svejda *et al.*, 1978). Benzimidazole and its derivatives also can be used as ligands in the field of coordination chemistry. The title compound was synthesized as part of our study of these ligands. Here we report the crystal structure of (I).



(I)

In the crystal structure of (I) (Fig. 1), the C—C and C—N bond lengths are similar to those found in 2-(2-ethoxyphenyl)-1-ethyl-1*H*-benzimidazole (Tong & Li, 2004) and its parent compound 2-(2-nitrophenyl)-1*H*-benzimidazole (Li *et al.*, 2005). The benzimidazole system is essentially planar, with a dihedral angle of 2.37 (16)° between the planes of the benzene ring and its fused imidazole ring. The whole molecule is non-planar; the benzimidazole ring makes an angle of 42.00 (15)° with the C8–C13 benzene ring.

In the crystal structure, the molecules of (I) are linked by N—H···N intermolecular hydrogen bonds (Table 1). The packing is further stabilized by van der Waals forces.

Experimental

A mixture of *o*-phenylenediamine (1.08 g, 0.01 mol) and 2,4-dichlorobenzaldehyde (3.50 g, 0.02 mol) was stirred in refluxing ethanol (30 ml) for 1 h to afford the title compound (3.8 g, yield 85%). The melting point of the product is 501–504 K. Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Crystal data

$C_{13}H_8Cl_2N_2$
M_r = 263.11
Orthorhombic, *Pbca*
a = 8.5630 (17) Å
b = 9.910 (2) Å
c = 28.694 (6) Å
V = 2435.0 (9) Å^3
Z = 8
D_x = 1.435 Mg m^{-3}
Mo *Kα* radiation
μ = 0.51 mm^{-1}
T = 295 (2) K
Block, yellow
0.30 × 0.20 × 0.15 mm

Data collection

Bruker P4 diffractometer
ω scans
Absorption correction: none
2602 measured reflections
2602 independent reflections
1316 reflections with $I > 2\sigma(I)$
$\theta_{max} = 27.0^\circ$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.156$
$S = 1.01$
2602 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0711P)^2 + 0.589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0018 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^{i}	0.86	2.06	2.866 (2)	155

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

H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H and C—H distances of 0.86 and 0.93 Å, respectively, and with U_{iso}(H) = 1.2U_{eq}(C,N) of the parent atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

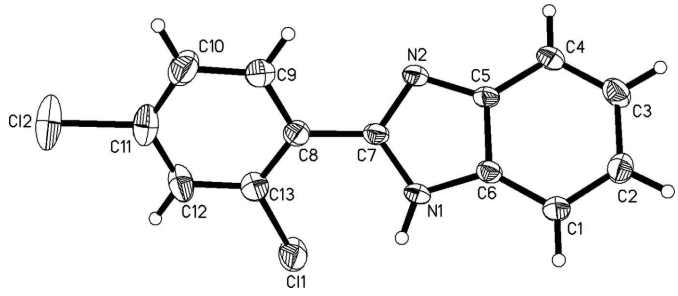


Figure 1
The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

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