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1-(2-Chlorobenzyl)-2-(2-chlorophenyl)-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 = 0.070
wR factor = 0.146
Data-to-parameter ratio = 15.6

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

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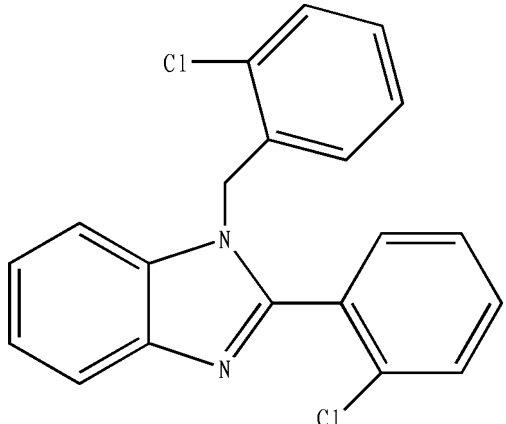
The title compound, $C_{20}H_{14}Cl_2N_2$, was prepared by reaction of *o*-phenylenediamine with 2-chlorobenzaldehyde under reflux in ethanol. The crystal structure is stabilized by van der Waals interactions.

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 can also 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 molecular 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 *et al.*, 2004) and its parent compound, 2-(2-nitrophenyl)-1*H*-benzimidazole (Li *et al.*, 2005). The dihedral angles between the least-squares plane of the benzimidazole group and those of the 2-chlorobenzyl and 2-chlorophenyl groups are 87.43 (1) and 71.58 (1)°, respectively. The 2-chlorobenzyl and 2-chlorophenyl groups make an angle of 80.87 (1)° with each other.

The crystal structure is stabilized by van der Waals interactions. No classical hydrogen-bond interactions or $\pi-\pi$ stacking interactions are found.

Experimental

A mixture of *o*-phenylenediamine (0.1 mol) and 2-chlorobenzaldehyde (0.2 mol) was stirred in refluxing ethanol (30 ml) for 1 h to afford the title compound (yield 85%). Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

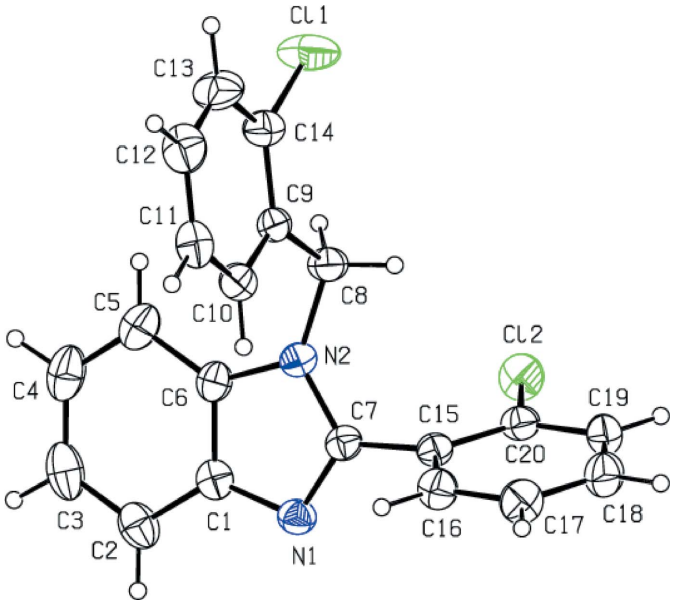


Figure 1
The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

Crystal data

$C_{20}H_{14}Cl_2N_2$
M_r = 353.23
Triclinic, $P\overline{1}$
a = 9.1302 (18) Å
b = 9.6848 (19) Å
c = 10.862 (2) Å
α = 90.29 (3)°
β = 98.89 (3)°
γ = 115.61 (3)°
V = 852.9 (4) Å^3
Z = 2
D_x = 1.375 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 295 (2) K
Block, yellow
0.25 × 0.20 × 0.15 mm

Data collection

Bruker P4 diffractometer
ω scans
3969 measured reflections
3388 independent reflections
3113 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 27.1°
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.146
S = 1.24
3388 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.5463P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

The H atoms were placed at calculated positions (C—H = 0.93 Å for aromatic H atoms and 0.97 Å for methylene H atoms) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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).

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