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# 3-Benzylidene-1-(2,6-dichlorophenyl)indolin-2-one

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.042
*wR* factor = 0.107
Data-to-parameter ratio = 13.6

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



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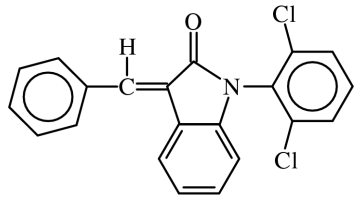
The phenyl and dichlorophenyl rings of the title molecule, $C_{21}H_{13}Cl_2NO$, are oriented at angles of 39.3 (1) and 77.8 (1)°, respectively, with respect to the central indoline ring. The crystal structure is stabilized by van der Waals interactions.

## Comment

Indole derivatives, widely distributed in living cells as tryptophan metabolites, have important biological functions. They are found to possess antihypertensive (Merk, 1971, 1974), anti-inflammatory (Rodriguez *et al.*, 1985) and antimalarial (El-Sayed *et al.*, 1986) activities. The structure determination of the title compound, (I), was undertaken to study the effect of the substituent groups on the conformation of the indoline ring and the molecular stereochemistry.




(I)

The phenyl ring is oriented at an angle of 39.3 (1)° with respect to the indoline ring. The dihedral angle between the dichlorophenyl ring and the indoline ring is 77.8 (1)°. The substituent groups at N1 and C2 of indoline do not disturb the planarity of that ring. The C*sp*$^2$—Cl bond lengths [C14—Cl1 = 1.725 (3) Å and C10—Cl2 = 1.728 (3) Å] are in good agreement with the literature values (Allen *et al.*, 1987). The exocyclic angle C2—C15—C16 of 129.5 (2)° deviates significantly from the normal value of 120°. This may be due to the repulsion between atoms H3 and H17 (2.31 Å). It is of interest to note that the shortest Cl···Cl intermolecular distance is 3.409 (2) Å, slightly smaller than the sum of the van der Waals radii of the corresponding atoms. The crystal structure is stabilized by van der Waals interactions.

## Experimental

A mixture of salicylaldehyde (0.01 mol), dichlorofenic acid (0.01 mol) and triethylamine (2 ml) was refluxed on an oil bath for 5 h. On cooling, a crystalline solid separated out, was filtered off and then washed with chilled methanol and recrystallized from ethanol (yield: 75%; m.p. 390–391 K).

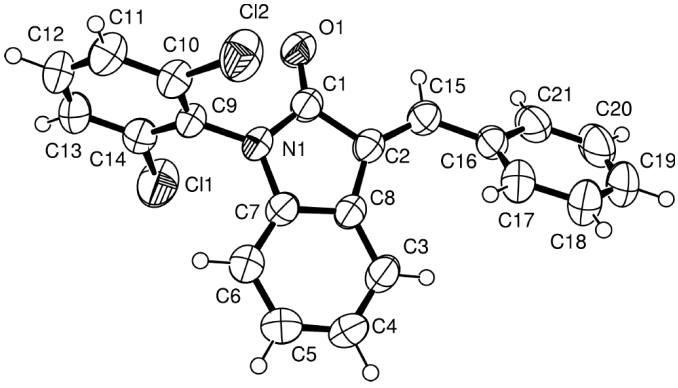



**Figure 1**
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

*Crystal data*

$C_{21}H_{13}Cl_2NO$
$M_r$ = 366.22
Monoclinic, $P2_1/n$
$a$ = 9.242 (5) Å
$b$ = 19.232 (12) Å
$c$ = 10.319 (5) Å
$\beta$ = 105.80 (4)°
$V$ = 1764.8 (17) Å$^3$
$Z$ = 4
$D_x$ = 1.378 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 10–15°
$\mu$ = 0.38 mm$^{-1}$
$T$ = 293 (2) K
Plate, white
0.30 × 0.25 × 0.20 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega$–2$\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.896, $T_{max}$ = 0.929
3290 measured reflections
3090 independent reflections
2276 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.013
$\theta_{max}$ = 25.0°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 22$
$l = -12 \rightarrow 11$
2 standard reflections
every 100 reflections
intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
$S$ = 1.11
3090 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2 + 1.0794P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0058 (8)

The H atoms were placed at geometrically calculated positions and a riding model was used for their refinement, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}$ of the attached atom.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *WinGX* (Farrugia, 1999); software used to prepare material for publication: *SHELXL*97.

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