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(3*E*)-3-[(4-Butylphenyl)imino]-1,3-dihydro-2*H*-indol-2-one

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.128
Data-to-parameter ratio = 15.4

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

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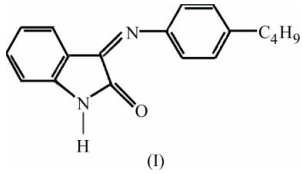
The title compound, $C_{18}H_{18}N_2O$, has a non-planar conformation. The indol and butylphenyl groups are connected by a C—N bond [1.433 (3) Å]. The crystal structure is stabilized by intermolecular N—H···N and C—H···O interactions.

Comment

Isatin and its derivatives have been used as reagents in the dye industry. Schiff bases of isatin were reported to possess anti-HIV (Pandeya *et al.*, 2000), antifungal (Pandeya *et al.*, 1999), antibacterial (Sarangapani & Reddy, 1994; Varma & Nobles, 1975), antiviral (Singh *et al.*, 1983), antiprotozoal (Varma & Khan, 1977) and antihelminthic (Sarciron *et al.*, 1993) activities. The medical and biological implications of this category of ligands has already been proved (Popp & Pajouhesh, 1982).



(I)

The structure of the title compound, (I), is shown in Fig. 1. The C1—C2 bond length [1.529 (3) Å] is within the range 1.49–1.56 Å observed for related compounds found in the Cambridge Structural Database (Allen, 2002). The C2—N2—C9 angle is 119.6 (2)°. In the butyl group, the average C—C—C bond angle is 114.7 (3)° and this group shows an *E* form. The indole group is planar [maximum displacement is 0.004 (2) Å for C1] and forms a dihedral angle of 89.8 (1)° with the phenyl plane. These bond distances and angles agree with the values reported for (3*E*)-3-[(4-hexylphenyl)imino]-1*H*-indol-2(3*H*)-one (Öztürk *et al.*, 2003).

The N—H···N and C—H···O hydrogen bonds form zigzag chains, parallel to the *b* axis (Fig. 2). The geometry of the hydrogen bonds is given in Table 2.

To determine the structural and electronic parameters of (I), quantum-chemical calculations were carried out using the *PM3* method (Stewart, 1985). It was found that the charges at atoms O1, N1 and N2 are 0.0382, 0.0609 and −0.2930 e$^-$, respectively. The final heat of formation of (I) is 14.98 kcal and its total energy is −3027.82 eV. The energies of the HOMO and LUMO levels have the values −9.0903 and −0.9315 eV, respectively. The calculated molecule dipole moment is 4.352 Debye.

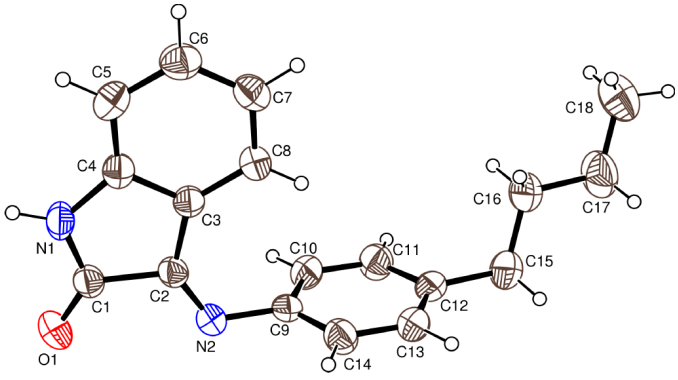


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

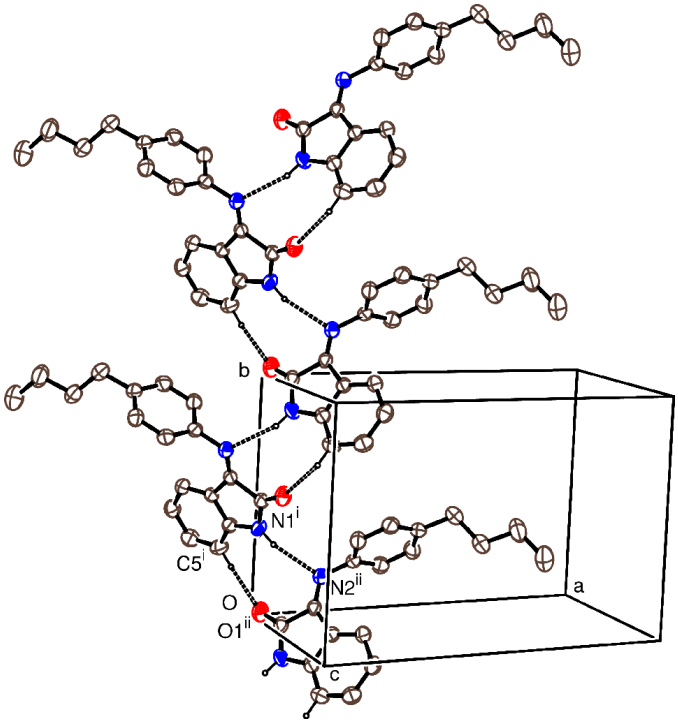


Figure 2
A view of the intermolecular hydrogen-bond contacts, showing the zigzag chain which develops parallel to *b*. [Symmetry codes: (i) $-x, -y, -z$; (ii) $x, \frac{1}{2}-y, \frac{1}{2}+z$.]

Experimental

The title compound was prepared according to the method of Öztürk *et al.* (2003). The orange product was recrystallized from methanol (m.p. 451–458 K).

Crystal data

$C_{18}H_{18}N_2O$	D_x = 1.232 Mg m^{-3}
M_r = 278.34	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 171 reflections
a = 15.6069 (2) Å	θ = 6.0–26.0°
b = 9.5596 (2) Å	μ = 0.08 mm^{-1}
c = 10.5265 (2) Å	T = 294 (2) K
β = 107.187 (2)°	Slab, orange
V = 1500.38 (5) Å^3	0.40 × 0.31 × 0.17 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	R_{int} = 0.072
ω scans	θ_{max} = 26.0°
Absorption correction: none	$h = -19 \rightarrow 19$
9152 measured reflections	$k = -11 \rightarrow 11$
2938 independent reflections	$l = -12 \rightarrow 12$
1851 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 0.2681P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.049	
$wR(F^2)$ = 0.128	
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
2938 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
191 parameters	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.214 (2)	C1—C2	1.531 (3)
N1—C1	1.356 (3)	C15—C16	1.524 (3)
N1—C4	1.413 (2)	C16—C17	1.502 (3)
N2—C2	1.272 (2)	C17—C18	1.504 (4)
N2—C9	1.433 (2)		
C1—N1—C4	111.73 (16)	C5—C4—N1	128.15 (18)
C2—N2—C9	119.60 (16)	C3—C4—N1	109.73 (17)
O1—C1—N1	128.03 (18)	C10—C9—N2	118.27 (18)
O1—C1—C2	125.99 (19)	C14—C9—N2	121.99 (19)
N1—C1—C2	105.91 (16)	C17—C16—C15	114.9 (2)
N2—C2—C3	135.31 (17)	C16—C17—C18	114.5 (2)
N2—C2—C1	118.87 (17)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{iii}	0.86	2.24	3.062 (2)	159
C5—H5···O1^{iii}	0.93	2.56	3.254 (3)	132

Symmetry code: (iii) $-x, \frac{1}{2}+y, \frac{3}{2}-z$.

The H atoms of C—H and N—H groups were placed in calculated positions (C—H = 0.96 Å and N—H = 0.86 Å) and were allowed to refine as riding models, with U_{iso} set equal to $1.2U_{eq}$ (1.5 for CH_3) of the carrier atoms.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *EVALCCD* (Duisenberg, 1998); data reduction: *EVALCCD*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997; Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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