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2-(2-Ethoxyphenyl)-1-ethyl-1*H*-benzimidazole

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The title compound, $C_{17}H_{18}N_2O$, was obtained by reaction of 2-(2-hydroxyphenyl)benzimidazole with bromoethane. The crystal structure is stabilized by intermolecular C—H$\cdots\pi$ interactions between the benzimidazole/benzimidazole and between the benzimidazole/phenolate moieties of adjacent molecules. No other hydrogen-bond interactions or π–π stacking interactions occur in the crystal packing, which is somewhat unusual for an aromatic heterocyclic compound.

Key indicators

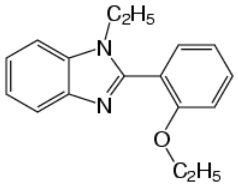
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.050
wR factor = 0.110
Data-to-parameter ratio = 10.5

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

Comment

Benzimidazole and its derivatives, such as 2-(2-hydroxyphenyl)benzimidazole and 2-(2-ethoxyphenyl)-1-ethyl-1*H*-benzimidazole, are excellent photoluminescent materials (Svejda *et al.*, 1978; Wu *et al.*, 2003). In recent years, more attention has been paid to their complexes and those of other similar *N*,*O*-donor ligands with metal ions and non-metal ions, such as Zn^{II}, Be^{II}, Al^{III}, Eu^{III} and B^{III}, because of their potential role as electroluminescent materials in organic light-emitting diodes (Wang, 2001; Huang *et al.*, 2002). These complexes are considered to be better electroluminescent materials than free ligands, owing to their increased thermal stability on coordination to metal or non-metal ions.

In an attempt to synthesize complexes of the ligand 2-(1-ethyl-1*H*-benzimidazol-2-yl)phenol with the metal ions mentioned above in order to obtain a blue-light emitter for further fabrication of electroluminescent diodes, we obtained another highly photoluminescent compound, (I), which emits strong blue light at room temperature. The crystal structure of (I) is reported here.



(I)

In the crystal structure of (I) (Fig. 1), the C—O and C—N bond lengths are similar to those found in related compounds, *e.g.* 2-(1*H*-benzimidazol-2-yl)-6-methoxyphenol (Elerman & Kabak, 1997), and the complexes of 2-(1*H*-benzimidazol-2-yl)-6-methylphenol with Co^{II} and Co^{III} (Crane *et al.*, 1999). However, in (I), the benzimidazole and phenolate moieties are almost perpendicular, owing to the steric hindrance arising from ethylation at the O and N positions with, for example, the C5—C6—C7—N2 torsion angle being −77.6 (3)°, which is quite different from the coplanarity observed for 2-(1*H*-

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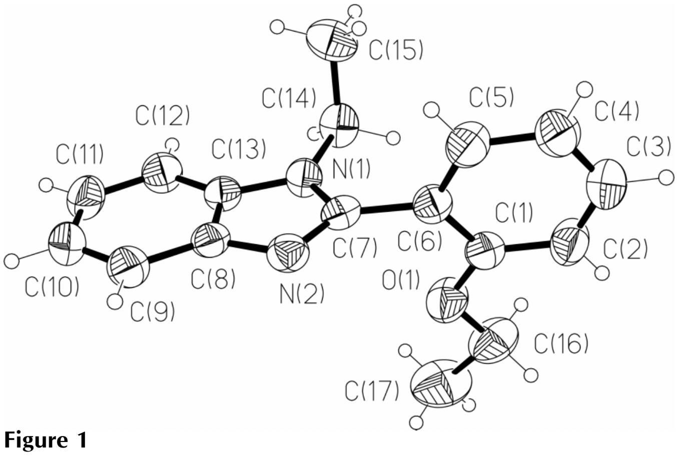

Figure 1
View of the molecule of (I). Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

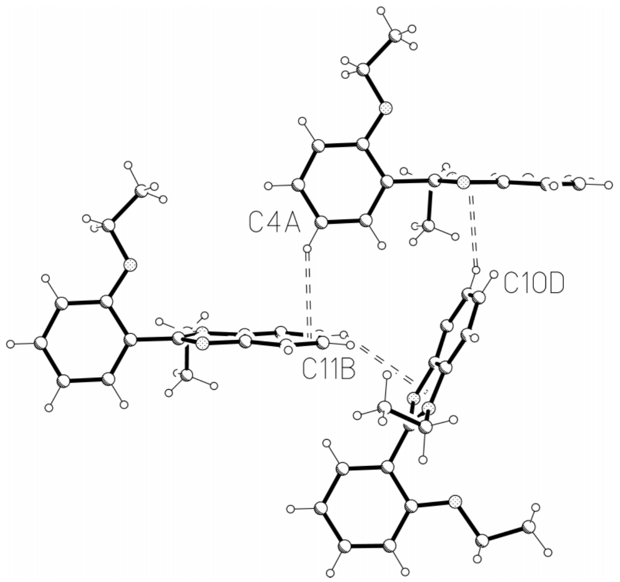

Figure 2
The C—H$\cdots\pi$ interactions (dashed lines) in the crystal packing of (I).

benzimidazol-2-yl)-6-methoxyphenol (Elerman & Kabak, 1997). Furthermore, this non-coplanarity, as well as the steric hindrance from the ethyl groups on the O and N positions, should block formation of intermolecular π–π stacking interactions. This is consistent with the observation of no intermolecular π–π stacking interactions in (I). However, C—H$\cdots\pi$ interactions (Srinivas *et al.*, 2004; Rodriguez *et al.*, 2004) occur between the benzimidazole/benzimidazole and between the benzimidazole/phenolate moieties of adjacent molecules (Fig. 2). These edge-to-face C—H$\cdots\pi$ interactions are somewhat different, with H$\cdots\pi$ distances of *ca* 2.82, 2.81 and 2.70 Å, and corresponding C—H$\cdots\pi$ angles of *ca* 151, 140 and 144°.

Experimental

The title compound, (I), was synthesized by a two-step reaction based on the method of Anthony & Philip (1981). Salicylic acid (0.138 g, 1 mmol) and *o*-phenylenediamine (0.108 g, 1 mmol) were mixed and stirred in syrupy phosphoric acid (3 ml) at a temperature of *ca* 520 K for 5 h to give white analytically pure 2-(2-hydroxyphenyl)benzimidazole after recrystallization of the crude product. The yield was *ca* 10%. 2-(2-Ethoxyphenyl)-1-ethyl-1*H*-benzimidazole was prepared by the reaction of 2-(2-hydroxyphenyl)benzimidazole and bromoethane under reflux conditions with a yield of *ca* 70%. The X-ray quality single crystal used in the structure determination was grown by slow evaporation of an ethanol solution for about one week. Analysis found: C 76.73, H 6.59, N 10.66%; calculated for $C_{17}H_{18}N_2O$: C 76.66, H 6.81, N 10.52%.

Crystal data

$C_{17}H_{18}N_2O$
$M_r = 266.33$
Orthorhombic, $P2_12_12_1$
$a = 9.3305$ (8) Å
$b = 12.4070$ (10) Å
$c = 12.7422$ (10) Å
$V = 1475.1$ (2) Å^3
$Z = 4$
$D_x = 1.199$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 1432 reflections
$\theta = 2.3$–20.8°
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Block, colorless
0.33 × 0.26 × 0.22 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.976$, $T_{\max} = 0.984$
9232 measured reflections

1922 independent reflections
1582 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 27.5°$
$h = -11 \rightarrow 11$
$k = -15 \rightarrow 16$
$l = -16 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.110$
$S = 1.08$
1922 reflections
183 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.2012P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C7	1.365 (3)	O1—C1	1.355 (3)
N1—C13	1.382 (3)	O1—C16	1.431 (4)
N1—C14	1.464 (3)	C14—C15	1.498 (4)
N2—C7	1.312 (3)	C16—C17	1.485 (5)
N2—C8	1.387 (3)		
C7—N1—C13	106.6 (2)	O1—C1—C2	124.9 (2)
C7—N1—C14	127.5 (2)	O1—C1—C6	115.3 (2)
C13—N1—C14	125.1 (2)	N1—C14—C15	111.8 (2)
C7—N2—C8	104.5 (2)	O1—C16—C17	107.8 (3)
C1—O1—C16	118.5 (2)		

H atoms were placed at calculated positions (C—H = 0.93 Å for all aromatic ring H atoms, 0.96 Å for all methyl H atoms and 0.97 Å for all methylene H atoms) and refined using the riding-model approximation, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ for aromatic ring and methylene H atoms, and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for all methyl H atoms. In the absence of significant anomalous dispersion effects, Friedel pair reflections were merged before the final refinement.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXL*97.

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