1-n-Butyl-2-(4'-fluorophenyl)-1H-benzimidazole-6-carbonitrile

The structure of the title compound, C\textsubscript{18}H\textsubscript{16}FN\textsubscript{3}, consists of neutral molecules. The asymmetric unit contains two independent molecules with similar conformations: the dihedral angles between the benzimidazole moiety and the benzene rings are 34.99 (9) and 36.08 (8)°. The crystal structure is stabilized by dipole–dipole and van der Waals interactions.

Comment

Benzimidazoles have pharmacological effects and are incorporated in many commercially available drugs (Sakai et al., 1989; Dubertret et al., 1999; Netland et al., 2000; Caro et al., 2001; Matsumori, 2003). Because of their antiparasitic and antiviral activities, new benzimidazoles have been synthesized and investigated for medical applications. Some of us have studied the syntheses and potent antifungal activities of a series of 5-cyanobenzimidazoles with substituted phenyl groups, and found that some of these compounds displayed wide antifungal activity against Candida sp., comparable to that of the commonly used antifungal, fluconazole (Goker et al., 2002). In this paper, we present the structure and stereochemical properties of a new cyanobenzimidazole, namely 1-n-butyl-2-(4'-fluorophenyl)-1H-benzimidazole-6-carbonitrile, (I) (Fig. 1).
related compounds (Bruno et al., 1996, 1997; Kendi et al., 1998, 1999; Özcan et al., 2000; Stibrany et al. 2003).
A packing diagram of (I) is shown in Fig. 2. There are no conventional hydrogen bonds and the crystal packing is dominated by van der Waals and dipole–dipole interactions between fluorine and the nitrogen of the CN group, resulting in the packing of the molecules in layers.

Experimental

The sodium metabisulphite adduct of 4-fluorobenzaldehyde (0.265 g, 1.25 mmol) was added to a suspension of 4-amino-3-n-butylamino-benzonitrile (0.19 g, 1 mmol) in DMF (5 ml), and heated at 383 K for 4 h. The reaction mixture was cooled and poured into water. The solid product was collected by filtration, washed with water and chromatographed with EtOAc–n-hexane (1:3). The final product was dissolved in ethanol and colourless crystals of (I) were grown by slow evaporation at room temperature.

Crystal data

C_{18}H_{16}FN_3

Mr = 293.34
Orthorhombic, Pca_2_1
a = 18.0843 (5) Å
b = 8.1980 (14) Å
c = 21.4690 (12) Å
V = 3182.9 (6) Å^3
Z = 8
D_x = 1.224 Mg m^{-3}

Data collection

Stoe IPDS-II diffractometer
\omega scans
Absorption correction: none
3216 independent reflections
1791 reflections with I > 2\sigma(I)
Mo Ka radiation
Cell parameters from 15 369 reflections
\theta = 0.00–24.7°
\mu = 0.08 mm^{-1}
T = 293 (2) K
Plate, colourless
0.40 × 0.32 × 0.06 mm

Refinement

Refinement on F^2
R[F^2 > 2\sigma(F^2)] = 0.036
wR(F^2) = 0.083
S = 1.00
3216 reflections
398 parameters
H-atom parameters constrained

w = 1/[\sigma^2(F_o^2) + (0.0453P)^2]
where P = (F^2 + 2F_c^2)/3
(D_max - D_min) = 0.12 e Å^{-3}
Extinction correction: SHELXL97
Extinction coefficient: 0.0088 (7)

H atoms were included using a riding model, with C–H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(methyl C). The Flack (1983) absolute structure parameter refined to an indeterminate value, and for the final cycles of refinement, Friedel pairs were merged.

Data collection: X-AREA (Stoe & Cie, 2002); cell refinement: X-AREA; data reduction: X-RED32 (Stoe & Cie, 2002); program(s) used to solve structure: SHELX97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

This work was financially supported by the Research Fund of Ondokuz Mayis University.
References