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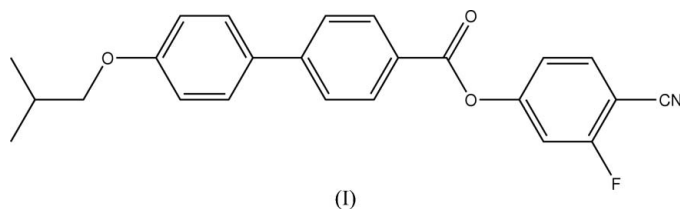
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.038
 wR factor = 0.097
Data-to-parameter ratio = 8.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.4-Cyano-3-fluorophenyl 4'-isobutoxybiphenyl-
4-carboxylate

In the title compound, $\text{C}_{24}\text{H}_{20}\text{FNO}_3$, the molecule is non-planar, with dihedral angles of 67.9 (1), 48.2 (1) and 20.3 (1)° between the three aromatic rings. The packing is stabilized by $\text{C}-\text{H}\cdots\pi$ and $\pi-\pi$ interactions.

Comment

Recently, liquid crystals including F atoms as substituents have become important because these molecules generally exhibit novel properties (Ozaki *et al.*, 1987; Wu *et al.*, 1992), such as low viscosity, high voltage percent retention and high specific resistance, when compared with the unsubstituted parent compounds. In our research on liquid crystal materials containing fluorine, we have synthesized the title compound, (I). We report its structure (Fig. 1) here.



The bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). The molecule is non-planar, and the three benzene rings make dihedral angles of 67.9 (1)° (angle between the C2–C7 and C9–C14 rings), 48.2 (1)° (angle between the C2–C7 and C15–C20 rings) and 20.3 (1)° (angle between the C9–C14 and C15–C20 rings). There exists a weak intramolecular $\text{C}23-\text{H}23\text{A}\cdots\text{O}3$ hydrogen bond, forming a five-membered ring (Table 2). In the crystal structure, the packing is stabilized by $\text{C}-\text{H}\cdots\pi$ (Table 2) and $\pi-\pi$ interactions involving the three benzene rings.

Experimental

To a solution of 4'-hydroxybiphenyl-4-carboxylic acid (1.0 g, 0.01 mol) in 6.4% KOH solution (10 ml) was added dropwise 1-bromo-2-methylpropane (3.22 g, 0.05 mol) in ethanol (30 ml). The mixture was refluxed for 90 h and extra KOH solution was added to remove the additional products. The mixture was then acidified to give a white precipitate, which was filtered and recrystallized from acetic acid, giving a white powder, identified as 4-isobutoxybiphenyl-4-carboxylic acid. This compound (0.75 g) and DCC (1,3-dicyclohexylcarbodiimide, 0.6 g) were dissolved in THF (20 ml), and a solution of 2-fluoro-4-hydroxybenzotrile (0.4 g) and DMAP (4-dimethylaminopyridine, 0.01 g) in THF (20 ml) was added. The mixture was stirred at 298 K for 140 h and then filtered. Colorless single crystals of (I) suitable for X-ray diffraction study were obtained by slow evaporation of an ethyl acetate/petroleum ether (1:7) solution, over a period of 10 d.

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Crystal data

C₂₄H₂₀FNO₃M_r = 389.41Orthorhombic, P2₁2₁2₁

a = 7.1969 (12) Å

b = 7.8499 (13) Å

c = 35.797 (6) Å

V = 2022.4 (6) Å³

Z = 4

D_x = 1.279 Mg m⁻³

Mo Kα radiation

Cell parameters from 4369 reflections

θ = 2.6–25.3°

μ = 0.09 mm⁻¹

T = 293 (2) K

Block, colorless

0.38 × 0.11 × 0.08 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.967, T_{max} = 0.993

11402 measured reflections

2315 independent reflections

2113 reflections with I > 2σ(I)

R_{int} = 0.020θ_{max} = 26.0°

h = -8 → 8

k = -9 → 9

l = -44 → 42

Refinement

Refinement on F²R[F² > 2σ(F²)] = 0.038wR(F²) = 0.097

S = 1.14

2315 reflections

262 parameters

H-atom parameters constrained

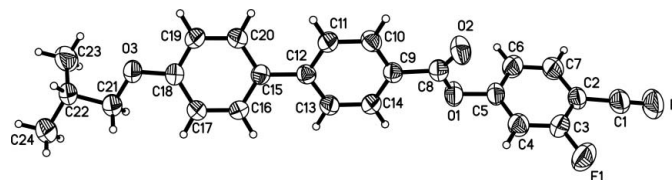
w = 1/[σ²(F_o²) + (0.0482P)² + 0.199P]where P = (F_o² + 2F_c²)/3(Δ/σ)_{max} = 0.006Δρ_{max} = 0.15 e Å⁻³Δρ_{min} = -0.14 e Å⁻³

Figure 1

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

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C–H distances in the range 0.93–0.98 Å, and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ (aromatic CH, methine CH and methylene CH₂) or $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ (methyl CH₃). The Friedel reflections were merged before the final refinement because of the absence of significant anomalous scattering effects.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST95 (Nardelli, 1995) and PLATON (Spek, 2003).

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Table 1

Selected bond lengths (Å).

F1–C3	1.345 (3)	O3–C18	1.370 (2)
O1–C8	1.366 (3)	O3–C21	1.431 (3)
O1–C5	1.403 (2)	N1–C1	1.137 (3)
O2–C8	1.188 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

D–H...A	D–H	H...A	D...A	D–H...A
C23–H23A...O3 ⁱ	0.96	2.55	2.891 (3)	101
C10–H10A...Cg3 ³	0.93	2.78	3.602	148
C14–H14A...Cg2 ⁱⁱ	0.93	2.92	3.725	146

Symmetry codes: (i) $-x - 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$. Cg2 and Cg3 are the centroids of rings C9–C14 and C15–C20, respectively.

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