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4-(Benzyloxy)-2-fluorobenzonitrile

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.074
wR factor = 0.244
Data-to-parameter ratio = 14.6

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

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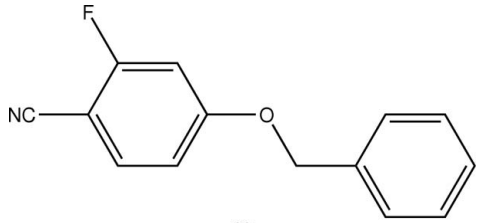
In the molecule of the title compound, $C_{14}H_{10}FNO$, the dihedral angle between the planar rings is 68.87 (4)°. The crystal structure is stabilized by C—H···π interations and π–π interactions.

Comment

Recently, liquid crystalline compounds containing fluorine atoms as substituents have become important because they 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 crystalline materials containing fluorine atoms, the title compound, (I), was synthesized and we report here its crystal structure.



(I)

In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings *A* (atoms C1–C6) and *B* (C8–C13) are, of course, planar and the dihedral angle between them is 68.87 (4)°.

The crystal structure (Fig. 2) is stabilized by C—H···π interactions (Table 1), and π–π interactions involving the benzene rings: *Cg*2···*Cg*2($-x$, $1-y$, $1-z$) = 3.805 Å, where *Cg*2 is the centroid of the C8–C13 ring.

Experimental

To a solution of 2-fluoro-4-hydroxybenzonitrile (2.74 g, 20 mmol) in KOH solution (17% *m*/*m*, 20 ml) was added dropwise a solution of

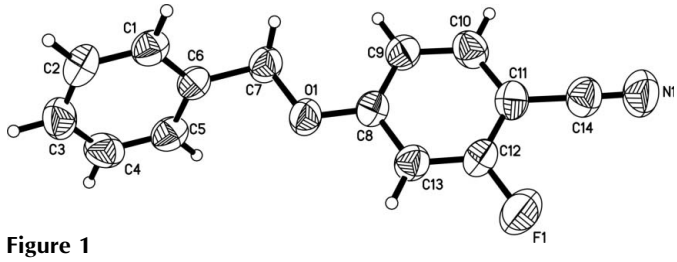


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

chloromethylbenzene (1.9 g, 150 mmol) in ethanol (50 ml). The mixture was refluxed for 24 h. An additional KOH solution (17.0% *m*/*m*, 10 ml) was added to remove the by-products. The mixture was then acidified to give a white precipitate, which was filtered off and recrystallized from ethanol, giving a white powder which was dried and then purified by column chromatography (ethyl acetate–petroleum ether, 1:4 *v*/*v*). Colorless single crystals of (I) suitable for X-ray diffraction analysis were obtained by slow evaporation of a solution in ethyl acetate–petroleum ether (1:2 *v*/*v*) over a period of 2 d.

Crystal data

$C_{14}H_{10}FNO$
M_r = 227.23
Monoclinic, $C2/c$
a = 23.420 (3) Å
b = 7.9307 (11) Å
c = 12.6046 (18) Å
β = 103.433 (2)°
V = 2277.1 (5) Å^3
Z = 8
D_x = 1.326 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, colorless
0.32 × 0.28 × 0.12 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.989
6209 measured reflections
2245 independent reflections
1605 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.244
S = 1.03
2245 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1426P)^2 + 2.351P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···$Cg1^{i}$	0.97	2.76	3.503	133

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

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

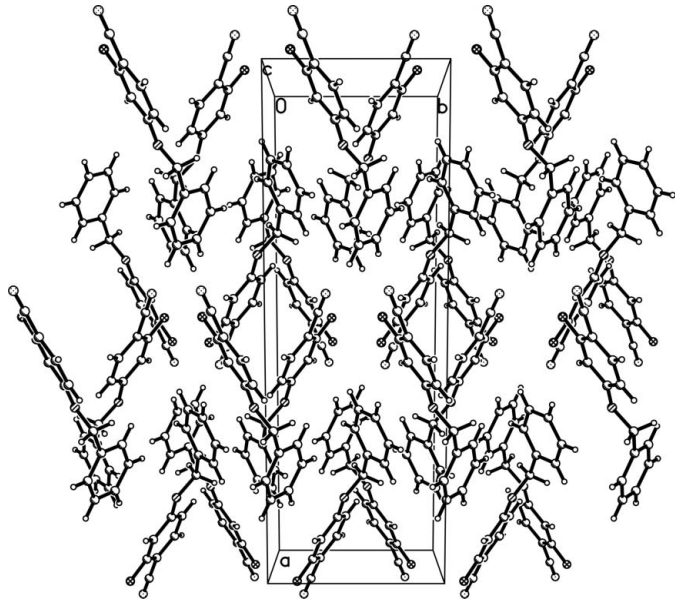


Figure 2
A packing diagram of (I).

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