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4-Cyano-3-fluorophenyl (2*E*)-3-(3-methoxy-4-octyloxyphenyl)acrylate

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Key indicators

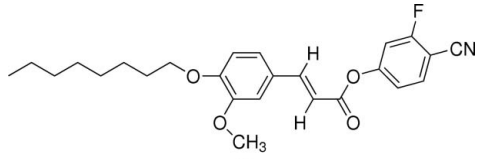
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.064
wR factor = 0.198
Data-to-parameter ratio = 15.6

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

In the title compound, $C_{25}H_{28}NO_4F$, the two aromatic rings are almost perpendicular with a dihedral angle of 84.6 (1)°. Molecules are linked into dimers by C—H···O interactions. The packing is further stabilized by π–π interactions.

Comment

We have recently reported the structure of 4-cyano-3-fluorophenyl (2*E*)-3-(4-heptyloxy-3-methoxyphenyl)acrylate (II) (Ren *et al.*, 2006). In order to investigate the effect of the length of the alkoxy linkage on liquid crystalline properties, the title compound, (I), was synthesized.



(I)

The bond lengths and angles in (I) are in good agreement with those in (II) (Ren *et al.*, 2006) and both compounds adopt similar conformations. The dihedral angle between the two benzene rings is 84.6 (1), while the C8—C9—C10—C11 torsion angle is 179.7 (3)° [the corresponding values in (II) are 87.7 (1) and 178.9 (2)°, respectively]. In (I), the F atom is disordered over two positions, with occupancies of 0.660 (5) and 0.340 (5). The intramolecular hydrogen bond, C10—H10*A*···O1, leads to the formation of a five-membered ring. In the crystal structure, molecules are linked into dimers *via* C—H···O interactions (Table 2, Fig. 2). The packing is further stabilized by π–π interactions involving the C2–C7 aromatic ring [$Cg1\cdots Cg1(2-x,-y,-z)$ = 3.778 Å, where *Cg*1 is the ring centroid].

Experimental

The title compound was synthesized by a similar method to that described by Ren *et al.* (2006). Colourless single crystals of (I)

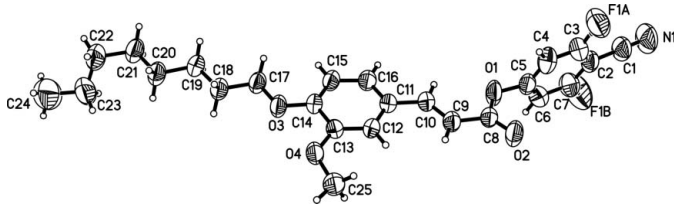


Figure 1
The structure of the compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The F atom is disordered over two positions, both of which are shown.

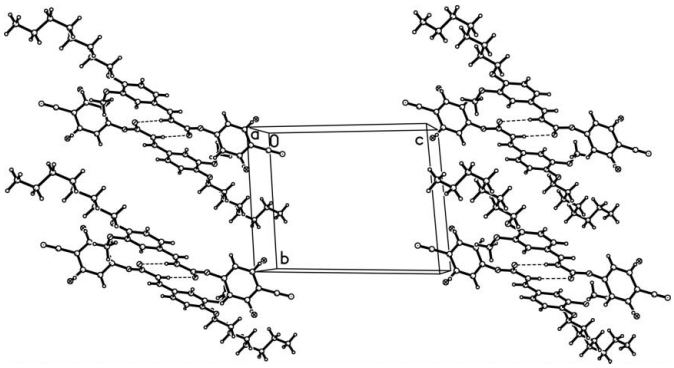


Figure 2
A view down the *a* axis of the unit cell, showing dimers. Hydrogen bonds are indicated by dashed lines.

suitable for X-ray diffraction studies were obtained by slow evaporation of a solution in a tetrahydrofuran/ethanol (1:4, *v*/*v*) solvent mixture over 2 d.

Crystal data

$C_{25}H_{28}FNO_4$
M_r = 425.48
Triclinic, $P\overline{1}$
a = 7.873 (4) Å
b = 11.279 (6) Å
c = 14.048 (7) Å
α = 81.016 (11)°
β = 80.419 (10)°
γ = 74.950 (10)°
V = 1179.5 (10) Å^3
Z = 2
D_x = 1.198 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1223 reflections
θ = 2.2–21.9°
μ = 0.09 mm^{-1}
T = 293 (2) K
Prism, colourless
0.19 × 0.14 × 0.09 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.984, T_{max} = 0.992
6504 measured reflections
4528 independent reflections
2364 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.2°
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 5$
$l = -17 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.198
S = 1.02
4528 reflections
290 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0887P)^2 + 0.167P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected bond lengths (Å).

F1*A*—C3	1.330 (4)	O3—C17	1.437 (3)
F1*B*—C7	1.276 (7)	O4—C13	1.372 (3)
O1—C8	1.357 (3)	O4—C25	1.418 (3)
O1—C5	1.385 (3)	N1—C1	1.135 (4)
O2—C8	1.194 (3)	C8—C9	1.448 (4)
O3—C14	1.357 (3)	C9—C10	1.327 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···O2^{i}	0.93	2.53	3.459 (4)	177
C10—H10*A*···O1	0.93	2.31	2.700 (3)	104

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

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms.

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*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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