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4-Cyano-3-fluorophenyl (2*E*)-3-(4-heptyloxyphenyl)acrylate

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Key indicators

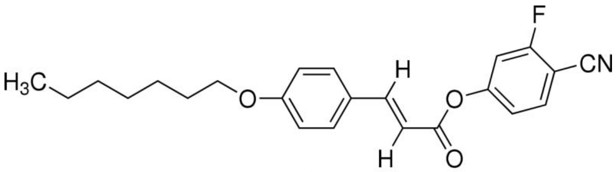
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.049
wR factor = 0.137
Data-to-parameter ratio = 15.6

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

In the title compound, $C_{23}H_{24}FNO_3$, the two benzene rings are inclined to one another by 41.2 (1)°. The double bond shows a *trans* configuration. The crystal packing is stabilized by dipole–dipole and van der Waals interactions.

Comment

We have reported previously the structure of 4-cyano-3-fluorophenyl (2*E*)-3-(4-heptyloxy-3-methoxyphenyl)acrylate, (I) (Ren *et al.*, 2006). In order to investigate the effect of the methoxy group on the conformation and liquid-crystal properties of (I), the title compound, (II), was synthesized and its crystal structure is reported here.



(II)

The molecular structure of (II) is illustrated in Fig. 1, and selected bond distances are given in Table 1. The bond lengths and angles in (II) are within normal ranges (Allen *et al.*, 1987), and agree well with the corresponding values in (I). The 4-heptyloxyphenyl group is essentially coplanar with the acrylate fragment, and the two benzene rings make a dihedral angle of 41.2 (1)° with one another. The double bond (C9═C10) shows a *trans* configuration, the C8—C9—C10—C11 torsion angle being 178.7 (1)°. The crystal packing is stabilized by dipole–dipole and van der Waals interactions.

Compound (II) also exhibits liquid-crystal properties. It has a melting point at 342 K and a clearing point at 397 K, and shows Schlieren texture in its liquid-crystalline phase.

Experimental

To a solution of 3-(4-hydroxyphenyl)acrylic acid (2.46 g, 15 mmol) in 16.0% NaOH solution (10 ml), 1-bromoheptane (0.54 g, 30 mmol) in ethanol (30 ml) was added dropwise. The mixture was heated under reflux for 24 h and extra NaOH solution was added to remove any by-products. The mixture was then acidified to give a white precipitate, which was filtered and recrystallized from ethanol, giving a white powder, identified as 3-(4-heptoxyphenyl)acrylic acid. This compound (1.31 g) and DCC (1,3-dicyclohexylcarbodiimide, 1.03 g) were dissolved in tetrahydrofuran (THF, 20 ml), and a solution of 2-fluoro-4-hydroxybenzonitrile (0.68 g) and DMAP (4-dimethylaminopyridine, 0.06 g) in THF (20 ml) was added. The mixture was stirred at room temperature for 24 h and then filtered. Colourless single crystals of (II), suitable for the X-ray diffraction study, were

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obtained by slow evaporation of a THF/ethanol (1:8 *v*/*v*) solution over a period of 5 d.

Crystal data

$C_{23}H_{24}FNO_3$
$M_r = 381.43$
Triclinic, $P\overline{1}$
$a = 7.5213$ (14) Å
$b = 10.507$ (2) Å
$c = 14.295$ (3) Å
$\alpha = 74.252$ (3)°
$\beta = 82.692$ (3)°
$\gamma = 70.764$ (3)°
$V = 1025.7$ (3) Å^3

$Z = 2$
$D_x = 1.235$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1979 reflections
$\theta = 2.3$–25.9°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Rod, colourless
0.34 × 0.22 × 0.11 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.971$, $T_{\max} = 0.991$
5802 measured reflections

3937 independent reflections
2888 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.014$
$\theta_{\max} = 26.1°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 10$
$l = -14 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.137$
$S = 1.04$
3937 reflections
253 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.1394P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

Table 1
Selected bond lengths (Å).

F1—C3	1.345 (2)	O3—C14	1.3583 (19)
O1—C8	1.3767 (19)	O3—C17	1.4352 (18)
O1—C5	1.3893 (19)	N—C1	1.137 (2)
O2—C8	1.1920 (19)	C9—C10	1.325 (2)

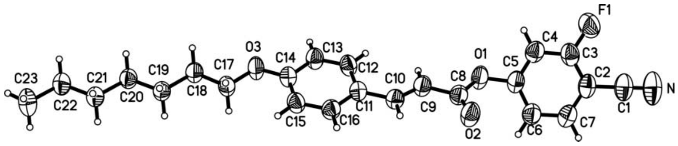

Figure 1
The molecular structure of compound (II), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

All H atoms could be located in difference Fourier maps but were included in calculated positions and treated as riding atoms, with C—H distances in the range 0.93–0.97 Å, and $U_{\rm iso}({\rm H}) = 1.2\,U_{\rm eq}$(parent C atom) or $U_{\rm iso}({\rm H}) = 1.5\,U_{\rm eq}$(methyl C atom).

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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