

5-(4-Fluoro-3-phenoxyphenyl)-3-(4-methylphenyl)-4,5-dihydroisoxazole

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Key indicators

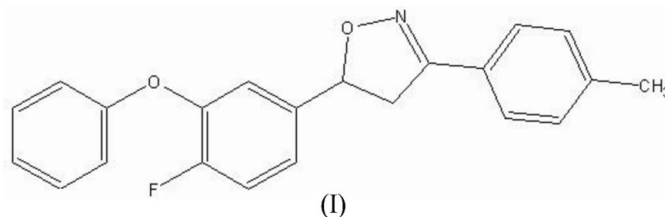
Single-crystal X-ray study
 $T = 290\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$
 R factor = 0.100
 wR factor = 0.219
Data-to-parameter ratio = 13.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the racemic crystal structure of the title chiral compound, $\text{C}_{22}\text{H}_{18}\text{FNO}_2$, the five-membered isoxazole ring has an envelope conformation with the chiral C atom at the flap position and deviating from the mean plane formed by the other four atoms by 0.319 (5) Å.

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Comment

Recent synthetic efforts have established the importance of biologically active heterocyclic compounds (Foti *et al.*, 2004). Of particular importance are the derivatives of isoxazoles representing one of the most active classes of compounds, widely used in agrochemicals and pharmaceuticals (He *et al.*, 2000). Such compounds have been studied from a synthetic (Bruno *et al.*, 2004) and also from a structural viewpoint (Zhong *et al.*, 2005). These have also been used in natural product synthesis and proven to be efficient precursors for many key synthetic intermediates, including γ -aminoalcohols, β -hydroxy ketons *etc.* (Kozikowski, 1984; Kanemasa & Tsuge, 1990). Spiro-oxazoles have exhibited herbicidal, plant-regulatory and antitumour activities (Howe & Shelton, 1990; De Amici *et al.*, 1990; Smietana *et al.*, 1999). In view of the important application of such a class of compounds and in continuation of our interest in the chemistry of isoxazoles we report here the crystal structure of title compound, (I).



Compound (I) is a functionalized isoxazole containing a methylphenyl group and a fluorophenoxyphenyl group attached to the five-membered heterocycle. The molecule contains a chiral C atom, C13 (Fig. 1). In spite of the presence of Csp^3 atoms C13 (chiral) and C15 in the molecule, the isoxazoline ring is approximately planar, the deviation of atom C13 being 0.319 (5) Å from the least-squares plane passing through O2/N1/C14/C15. This is because of the extended π conjugation involving the ring sp^2 -hybridized atom C14 and heteroatoms N1 and O2 (see the geometric parameters for bond lengths involving these atoms; Table 1). Furthermore, the methylphenyl and isoxazole rings make a dihedral angle of 5.9 (2)°, whereas the fluorophenoxy group is orthogonal to the five-membered ring, the dihedral angle being 72.6 (2)°. Puckering analysis of the five-membered isoxazole ring

(Cremer & Pople, 1975) indicates a total puckering amplitude $Q(2) = 0.200(4) \text{ \AA}$ and $\varphi(2) = 140(1)^\circ$ [$\varphi(2) = 36k$; envelope conformation, $k = 4$], indicating that the five-membered ring exists in an envelope conformation.

Experimental

Compound (I) was synthesized in accordance with the procedure reported in the literature (Joseph *et al.*, 2004; Archana *et al.*, 2002). Single crystals of (I) were obtained from a dichloromethane/hexane solution (2:1 v/v) of (I) at 276 (1) K.

Crystal data

$C_{22}H_{18}FNO_2$	$Z = 8$
$M_r = 347.37$	$D_x = 1.282 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation
$a = 10.565(7) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 8.274(6) \text{ \AA}$	$T = 290(2) \text{ K}$
$c = 41.17(3) \text{ \AA}$	Plate, colourless
$V = 3599(4) \text{ \AA}^3$	$0.40 \times 0.15 \times 0.02 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	23870 measured reflections
φ and ω scans	3159 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2067 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.948$, $T_{\max} = 0.998$	$R_{\text{int}} = 0.066$
	$\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0797P)^2 + 0.661P]$
$R[F^2 > 2\sigma(F^2)] = 0.100$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.219$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.32$	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
3159 reflections	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$
240 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

C14–N1	1.275 (5)	O2–C13	1.454 (5)
O2–N1	1.404 (4)	C7–O1	1.374 (5)
N1–C14–C15	113.0 (3)	C14–C15–C13	101.2 (3)
N1–O2–C13	108.2 (3)	O2–C13–C15	103.5 (3)
C17–C16–C14–C15	−178.5 (4)	C10–C11–C13–C15	74.8 (5)

H atoms were placed in calculated positions with C–H = 0.93–0.98 \AA . The torsion angle of the methyl group was refined to fit the electron density, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. Other H atoms were refined in riding mode; $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

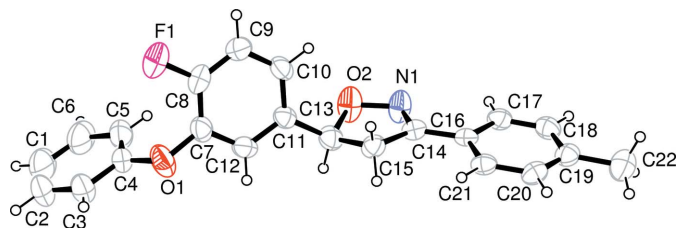


Figure 1

The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1999) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

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