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

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Key indicators

Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.007 Å
R factor = 0.100
wR factor = 0.219
Data-to-parameter ratio = 13.2

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

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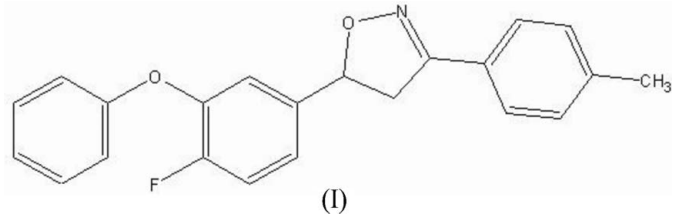
In the racemic crystal structure of the title chiral compound, $C_{22}H_{18}FNO_2$, the five-membered isoxazole ring has an envelope conformation with the chiral C atom at the flap position and deviating from the mean plane formed by the other four atoms by 0.319 (5) Å.

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).



(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) Å and $\varphi(2)$ = 140 (1)° [$\varphi(2) = 36k$; 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

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

Data collection

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

Refinement

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

Table 1
Selected geometric parameters (Å, °).

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 Å. The torsion angle of the methyl group was refined to fit the electron density, with U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were refined in riding mode; U_{iso}(H) = 1.2U_{eq}(C).

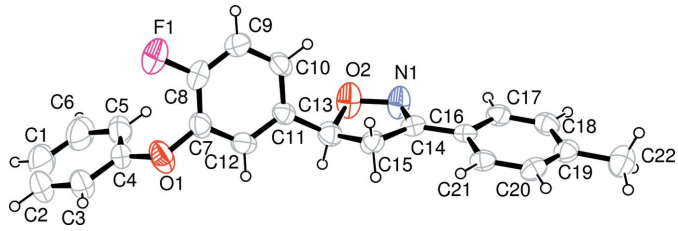


Figure 1
The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

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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