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2-(4-Fluorophenyl)-2-oxo-1-(1*H*-1,2,4-triazol-1-yl)ethyl piperidine-1-carbodithiolate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.086
Data-to-parameter ratio = 13.5

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

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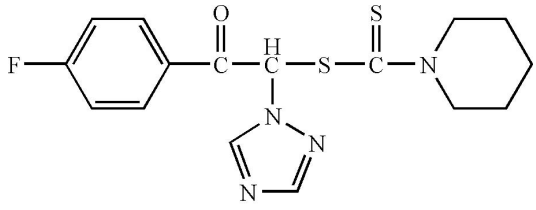
The molecule of the title compound, $C_{16}H_{17}FN_4OS_2$, is built up around a chiral C atom, and exists in a propeller-like arrangement. The structure is stablized by van der Waals interactions.

Comment

As an important type of fungicides, triazole compounds are highly efficient and of low toxicity (Shi *et al.*, 1995; Xu *et al.*, 2002). Triazole nuclei appear frequently in the structures of various natural products and biologically active compounds, notably thiamine (vitamin B), penicillins, antibiotics such as micrococcin (James *et al.*, 1966), and many metabolic products of fungi and primitive marine animals. Present studies of triazole derivatives concentrate mainly on compounds with triazole as the only active group, while reports of compounds containing both triazole and piperidine groups in a single molecule are scarce. We have therefore studied the title compound, (I), and present its structure here.



(I)

As shown in Fig. 1, the molecule of (I) is built up around the chiral atom C7, which is connected to a piperidine carbodithiolate, a triazole and a fluorophenyloxo group, in a propeller-like arrangement. The four atoms S1, S2, N1 and C1 (*p*1) of the carbodithiolate are planar, as are the triazole and fluorophenyl groups. The dihedral angles between *p*1 and the triazole and fluorophenyl groups are 66.69 (8) and 81.89 (7)°, respectively. The dihedral angle between the triazole and fluorophenyl groups is 67.88 (4)°.

The bond lengths and angles in the 1,2,4-triazole and phenyl rings are generally normal (Ji *et al.*, 2002; Allen *et al.*, 1987). The bond lengths and angles within the piperidine ring are also in good agreement with the earlier report by Yuan *et al.* (2004). The C—F bond length [1.357 (2) Å] is similiar to that found by Lynch & McClenaghan (2004) [1.340 (3)–1.345 (3) Å].

There are some weak C—H···S intramolecular hydrogen bonds (Table 1) (Song *et al.*, 2003). The packing is stabilized by weak van der Waals interactions.

Experimental

The title compound was prepared by the reaction of 2-bromo-1-(4-fluorophenyl)-2-(1*H*-1,2,4-triazol-1-yl)ethanone (0.02 mol, 5.7 g), piperidine (0.02 mol, 1.7 g), CS_2 (0.02 mol, 1.5 g) and potassium hydroxide (0.02 mol, 1.1 g) in ethanol solution at room temperature. Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from chloroform at room temperature.

Crystal data

$C_{16}H_{17}FN_4OS_2$
M_r = 364.46
Triclinic, $P\overline{1}$
a = 8.7112 (15) Å
b = 9.8967 (17) Å
c = 11.1551 (19) Å
α = 73.323 (2)°
β = 88.603 (2)°
γ = 66.981 (2)°
V = 843.7 (3) Å^3
Z = 2
D_x = 1.435 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1376 reflections
θ = 2.5–24.1°
μ = 0.34 mm^{-1}
T = 295 (2) K
Block, colourless
0.24 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.910, T_{max} = 0.948
4609 measured reflections
2932 independent reflections
2231 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 25.0°
$h = -9 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.086
S = 1.10
2932 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.0282P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2*A*···S1	0.97	2.53	3.052 (3)	114
C6—H6*B*···S2	0.97	2.39	2.939 (2)	115
C7—H7···S1	0.98	2.45	3.108 (3)	124
C12—H12···S1	0.93	2.81	3.735 (2)	172

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances in the range 0.93–0.97 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

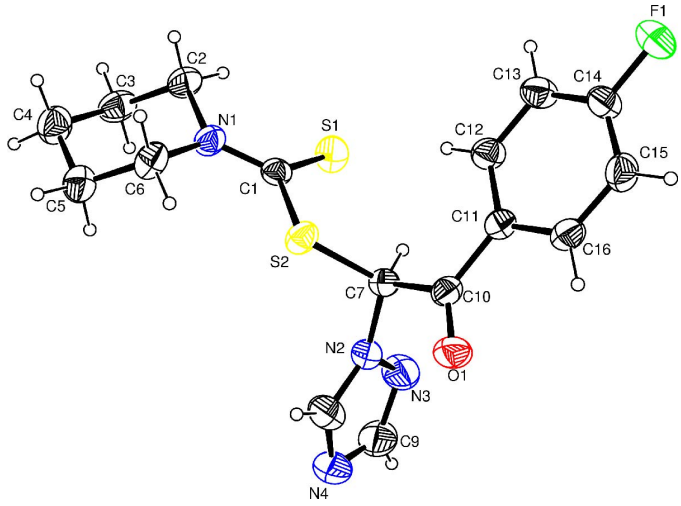


Figure 1
The structure of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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