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1-(2,4-Difluorophenyl)-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one

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In the crystal structure of the title compound, $C_{11}H_9F_2N_3O$, dimers are formed *via* C—H···O hydrogen bonding. These dimers are located around centres of inversion.

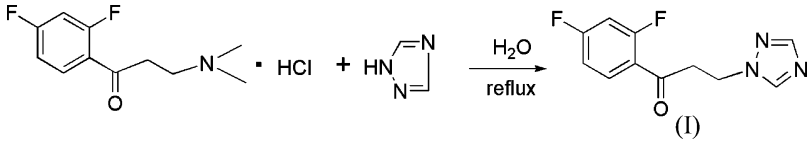
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.126
Data-to-parameter ratio = 12.3

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

Comment

It is well known that compounds containing the triazole ring have good fungicidal and plant growth-regulating activities (Konosu *et al.*, 2001; Miyauchi *et al.*, 1995; Dyck *et al.*, 2003; Sekimata *et al.*, 2002; Ruel *et al.*, 2003). We report here the crystal structure of the title compound, (I) (Fig.1).



(I)

Bond lengths and angles of (I) are within normal ranges (Allen *et al.*, 1987) and are comparable with those in a related compound (Wan *et al.*, 2005). The molecule of (I) is non-planar, with the benzene and triazole rings making a dihedral angle of 50.6 (2)°.

The crystal structure of (I) is stabilized by an intermolecular C11—H11···O1 hydrogen bond [H11···O1 = 2.36 Å, C11···O1 = 3.245 (3) Å and C11—H11···O1^{i} = 160°; symmetry code: (i) $-x+2, -y+1, -z+2$] (Fig. 2).

Experimental

The title compound was prepared according to the method reported by Ehrhardt *et al.* (1982). 1*H*-1,2,4-Triazole (0.15 mol, 10.35 g) was dissolved in water (20 ml). The mixture was heated to reflux and kept at this temperature for 1 h, and then a solution of 1-(2,4-difluorophenyl)-3-(dimethylamino)propan-1-one hydrochloride (0.14 mol, 34.9 g) in water (45 ml) was added dropwise over a period of 2 h to the above heated mixture. After the addition, the reaction mixture was stirred at reflux for a further 2 h and then cooled to room temperature. A white solid was collected, which was recrystallized from ethyl acetate to give colourless crystals of (I) (yield 82%).

Crystal data

$C_{11}H_9F_2N_3O$
M_r = 237.21
Triclinic, $P\overline{1}$
a = 6.939 (3) Å
b = 7.743 (4) Å
c = 10.939 (5) Å
α = 100.685 (7)°
β = 90.650 (8)°
γ = 110.307 (7)°
V = 539.8 (4) Å^3
Z = 2
D_x = 1.459 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 294 (2) K
Block, colourless
0.22 × 0.20 × 0.18 mm

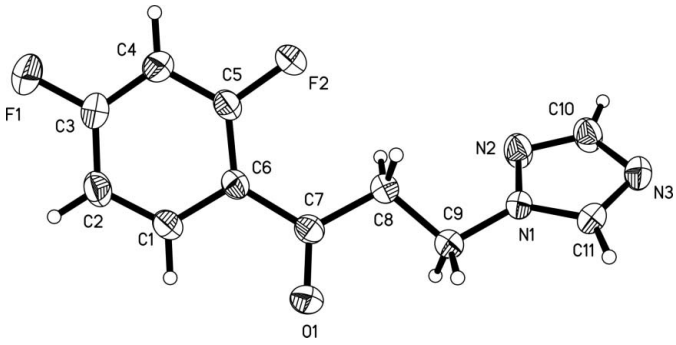


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

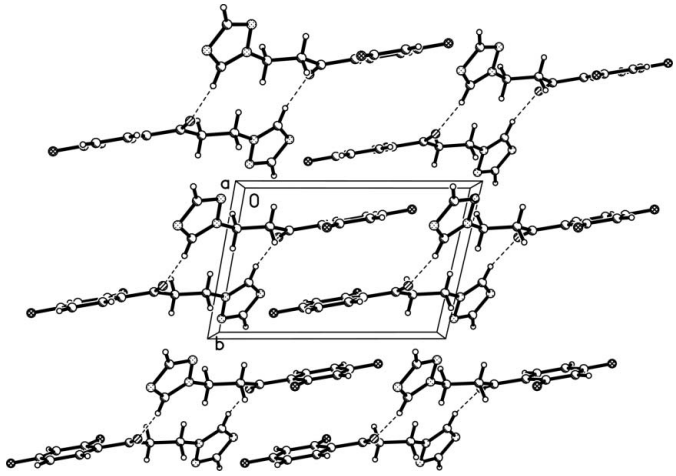


Figure 2
A packing diagram of the title compound. Dashed lines indicate C—H···O hydrogen-bond interactions.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.974, T_{max} = 0.979
2748 measured reflections
1897 independent reflections
1316 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.126
S = 1.03
1897 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2 + 0.0629P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

All H atoms were placed in calculated positions, with C—H = 0.93 and 0.97 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); 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: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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