Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

3-Benzyloxy-6-fluoropyridazine

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Received 13 June 2005
Accepted 16 June 2005
Online 24 June 2005

Key indicators

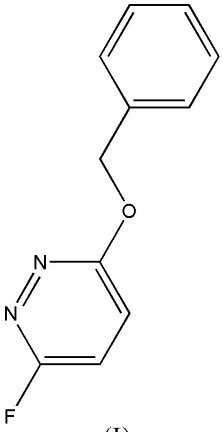
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.053
wR factor = 0.162
Data-to-parameter ratio = 14.8

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

The title molecule, $C_{11}H_9FN_2O$, was synthesized from 3,6-difluoropyridazine, benzyl alcohol and sodium hydroxide in CH_3CN under reflux. The asymmetric unit contains two independent molecules with nearly identical geometry. In the crystal structure, the molecules are linked by weak intermolecular C—H$\cdots$F hydrogen bonds and C—H$\cdots\pi$ interactions.

Comment

Pyridazine derivatives are very attractive because of their varied bioactivity. For example, maleic hydrazide, pyrazon and norflurazon are widely used as herbicides. In addition, some of them possess pesticidal activity (Endo *et al.*, 2000), antiviral activity (Raymond *et al.*, 1991) and plant-growth regulating activity (Matsumoto & Ishitani, 1988). This led us to pay more attention to the synthesis and structure determination of these compounds. Recently, we synthesized a series of pyridazine derivatives to study the relationship between structure and herbicidal activity. We report here the crystal structure of the title compound, (I).



(I)

The asymmetric unit of (I) contains two independent molecules (Fig. 1); the geometry of these two molecules is nearly identical. The dihedral angle between planes C1–C4/N1/N2 and C6–C11 is 31.8 (1)°, and that between planes C12–C15/N3/N4 and C17–C22 is 28.1 (2)°. The C4—O1—C5—C6 and C15—O2—C16—C17 torsion angles are 172.0 (3) and 171.8 (4)°, respectively. In the crystal structure, the two independent molecules are linked through a C—H$\cdots\pi$ interaction involving the C6–C11 benzene ring (centroid Cg1). A weak intermolecular C—H$\cdots$F hydrogen bond is also observed (Table 1).

doi:10.1107/S1600536805019161

Experimental

The title compound was synthesized according to the reported procedure of Yang *et al.* (2002), by refluxing 3,6-difluoropyridazine (0.24 g, 2.06 mmol), benzyl alcohol (0.22 g, 2.03 mmol) and sodium hydroxide (0.10 g, 2.50 mmol) in acetonitrile (20 ml) for 2 h. After cooling, the reaction mixture was poured into water. The precipitate was filtered off and recrystallized from petrolum ether, giving single crystals suitable for X-ray diffraction.

Crystal data

$C_{11}H_9FN_2O$
M_r = 204.20
Monoclinic, $P2_1/c$
a = 29.409 (4) Å
b = 5.8286 (14) Å
c = 11.730 (3) Å
β = 101.220 (8)°
V = 1972.3 (7) Å^3
Z = 8
D_x = 1.375 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1457 reflections
θ = 2.8–20.8°
μ = 0.10 mm^{-1}
T = 294 (2) K
Prism, colourless
0.40 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.950, $T_{\max}$ = 0.990
11179 measured reflections
4027 independent reflections
1718 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.072
$\theta_{\max}$ = 26.4°
$h = -36 \rightarrow 36$
$k = -4 \rightarrow 7$
$l = -14 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.162
S = 0.98
4027 reflections
273 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2 + 0.0302P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.19 e Å^{-3}
$\Delta\rho_{\min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.0057 (11)

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

Cg1 is the centroid of the C6–C11 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···F1$^{\rm i}$	0.93	2.54	3.350 (5)	146
C20—H20···*Cg*1	0.93	3.07	3.723 (6)	128

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

The structure is twinned (twin matrix $10 1/0\bar{1}0/00\bar{1}$), with a twinning factor of 0.291 (2). All H atoms were placed in calculated positions, with C—H distances of 0.93 or 0.97 Å, and included in the final cycles of refinement using a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(parent atom).

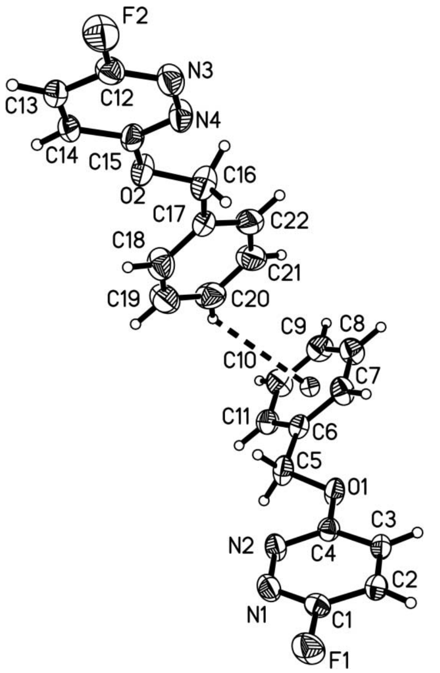


Figure 1
The asymmetric unit of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme. The dashed line represents the C—H···π interaction.

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

The authors acknowledge the financial support of the National Natural Science Foundation of China (grant No. 20302004) and the Doctors' Special Foundation of the Higher Education Ministry (grant No. 20020055022).

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