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5-(4-Fluorobenzylidene)imidazolidine-2,4-dione

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.040
wR factor = 0.114
Data-to-parameter ratio = 6.8

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

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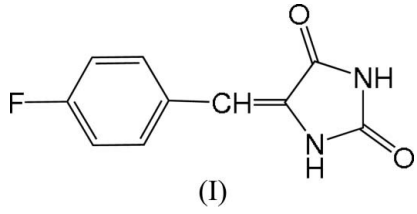
The title compound, $C_{10}H_7FN_2O_2$, was synthesized by the reaction of 4-fluorobenzaldehyde and imidazolidine-2,4-dione under microwave irradiation. In the crystal structure, there are intermolecular N—H···O hydrogen bonds and weak π–π interactions.

Comment

Imidazolidine-2,4-diones represent an important class of five-membered heterocycles. Some derivatives of imidazolidine-2,4-diones have intrinsic germicidal (Marton *et al.*, 1993) and anticonvulsant (Wong & Tan, 1989) properties and have been used to synthesize unnatural amino acids by transamination (Nagasaki *et al.*, 1973). We report here the microwave-assisted synthesis and the crystal structure of the title compound, (I). The molecular structure and packing of (I) are shown in Figs. 1 and 2, respectively, where the dashed lines indicate intermolecular N—H···O hydrogen bonds (Table 2). A planar chain structure of (I) held together by intermolecular hydrogen bonds is shown in Fig. 2. The weak π–π interaction is shown in Fig. 3; *Cg*1 is the centroid of atoms C1–C6, and *Cg*2 is the centroid of atoms C8/N2/C9/C10/N1. The inter-centroid distance between layers is 3.8250 (8) Å. The bond lengths and angles are given in Table 1. Full details of the hydrogen bonding are given in Table 2.



(I)

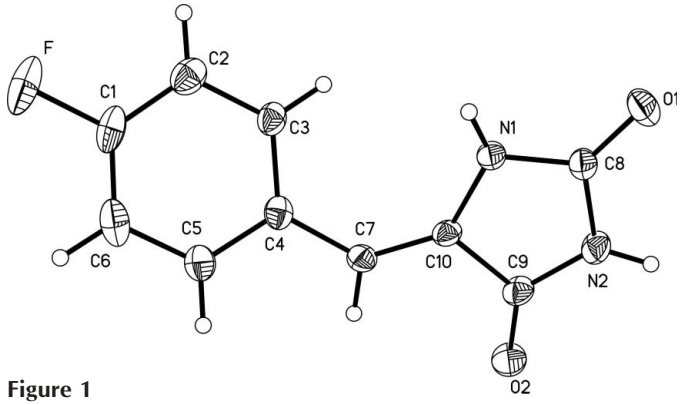


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

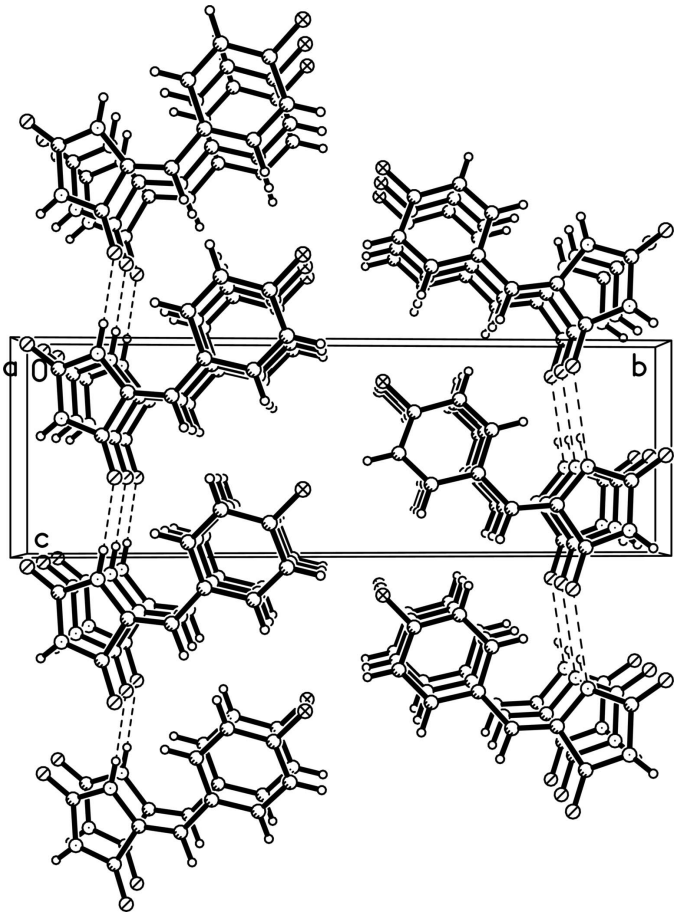


Figure 2
A packing diagram of the molecular structure of (I), viewed along the *a* axis; broken lines indicate intermolecular N—H···O hydrogen bonds.

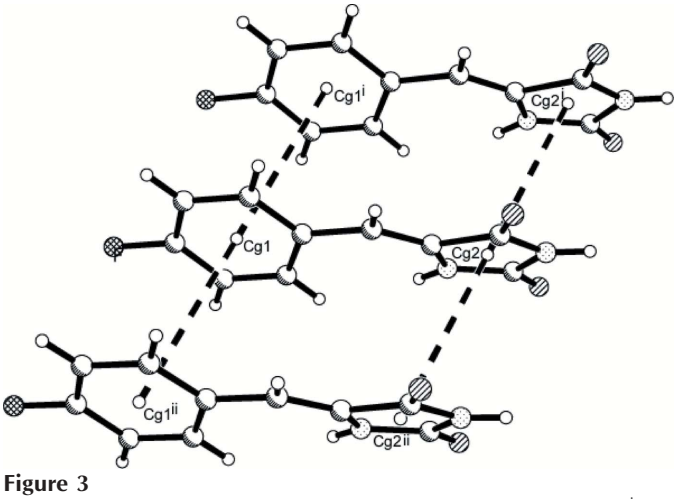


Figure 3
Weak π–π interactions in (I); the inter-centroid distances, $Cg1\cdots Cg1^{i}$ and $Cg2\cdots Cg2^{i}$, are both 3.8250(8) Å. [Symmetry codes: (i) $1+x, y, z$; (ii) $-1+x, y, z$.]

Experimental

4-Fluorobenzaldehyde (10 mmol) and imidazolidine-2,4-dione (10 mmol) were dissolved in water (10 ml) and ethanolamine (0.1 ml) was added in one portion. The resulting mixture was refluxed for 5 min under microwave irradiation, then filtered under reduced pressure and washed with ethanol (10 ml) to afford crude compound (I). Pure compound (I) was obtained by crystallization from glacial acetic acid (20 ml). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a glacial acetic acid solution.

Crystal data

$C_{10}H_7FN_2O_2$
M_r = 206.18
Monoclinic, $P2_1$
a = 3.8250 (8) Å
b = 6.2410 (12) Å
c = 18.988 (4) Å
β = 95.25 (3)°
V = 451.38 (16) Å^3
Z = 2
D_x = 1.517 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9–12°
μ = 0.12 mm^{-1}
T = 293 (2) K
Thick plate, light yellow
0.3 × 0.2 × 0.1 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1155 measured reflections
985 independent reflections
806 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 26.0°
$h = 0 \rightarrow 4$
$k = -1 \rightarrow 7$
$l = -22 \rightarrow 22$
3 standard reflections every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.114
S = 1.06
985 reflections
145 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.064P)^2 + 0.038P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.026 (9)

Table 1
Selected geometric parameters (Å, °).

F—C1	1.371 (5)	N2—C9	1.354 (5)
O2—C9	1.220 (5)	N2—C8	1.396 (5)
O1—C8	1.209 (4)	C1—C2	1.361 (6)
C10—C7	1.339 (4)	C2—C3	1.376 (5)
C10—N1	1.388 (5)	C3—C4	1.400 (5)
C10—C9	1.487 (5)	C4—C7	1.459 (5)
N1—C8	1.361 (5)		
C7—C10—N1	133.4 (3)	C3—C4—C7	123.2 (3)
C7—C10—C9	122.0 (3)	C10—C7—C4	131.5 (4)
N1—C10—C9	104.5 (3)	O1—C8—N1	127.2 (4)
C8—N1—C10	111.3 (3)	O1—C8—N2	125.9 (4)
C9—N2—C8	111.0 (3)	N1—C8—N2	107.0 (3)
C2—C1—F	118.0 (5)	O2—C9—N2	126.8 (4)
C6—C1—F	119.0 (4)	O2—C9—C10	127.0 (4)
C5—C4—C7	118.8 (4)	N2—C9—C10	106.2 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.83 (4)	2.05 (4)	2.865 (4)	166 (4)
N2—H2···O1^{ii}	0.88 (4)	1.93 (4)	2.797 (4)	170 (5)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, y+\frac{1}{2}, -z$.

No attempt has been made to establish the polarity of the crystal, as no significant anomalous dispersion at this wavelength is expected; Friedel pairs were merged. All H atoms bonded to C atoms were positioned geometrically at a C—H distance of 0.93 Å and included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.5U_{eq}$ of the carrier atom. All H atoms bonded to N atoms were located in a difference Fourier synthesis and refined freely.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *PLATON* (Spek, 2003).

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