ORGANIC COMPOUNDS

Acta Cryst. (1996). C**52**, 2771–2772

3-Benzyl-5-(2-fluorobenzylidene)-imidazolidine-2,4-dione

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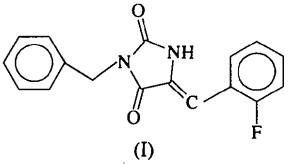
(*Received 20 November 1995; accepted 4 June 1996*)

Abstract

The title compound, $C_{17}H_{13}FN_2O_2$, has a dihedral angle of 160.5 (1)° between the fluorobenzylidene and the imidazolidinedione rings with an angle of 109.3 (1)° between the latter ring and the benzyl ring. The molecules are linked by an N—H···O hydrogen bond [N···O 2.852 (3) Å].

Comment

The title compound, (I), belongs to a class of imidazolidine and thiazolidine derivatives that show different pharmacological activities including antibacterial, antifungal and insecticidal activity (Labouta, Salama, Eshba, Kader & El-Chrbini, 1987). As the knowledge of its stereochemistry may aid the understanding of its pharmacological behaviour, a crystal structure determination of (I) was undertaken.



(I)

The benzyl, imidazolidinedione and fluorobenzylidene rings are planar within experimental accuracy, as shown by the values of σ_{av} [defined as $(\Sigma d_i^2/N - 3)^{1/2}$] which are 0.004, 0.010 and 0.004 Å, respectively.

The dihedral angle between the fluorobenzylidene and the imidazolidinedione rings is 160.5 (1)° and that between the latter ring and the benzyl ring is 109.3 (1)°. The exocyclic angles around N1 are greater than the endocyclic angle; however, the sum of the valency angles around N1 is 359.9°, indicating no significant pyramidalization of this atom. The overall geometry of the five-membered ring is in good agreement, to within experimental accuracy, with that found in the literature (De Bondt, Blaton, Peeters & De Ranter, 1994; Bruno *et al.*, 1994; Olszak, Peeters, Blaton & De Ranter, 1994*a*,*b*).

The molecules are linked by a hydrogen bond [N2···O1^{i} = 2.852 (3), HN2···O1^{i} = 1.94, N2—HN2 = 0.95 Å, N2—HN2···O1^{i} = 162°; (i) = $1-x, -y, 1-z$].

A *ZORTEP* (Zsolnai, 1995) illustration of the formula unit is presented in Fig. 1.

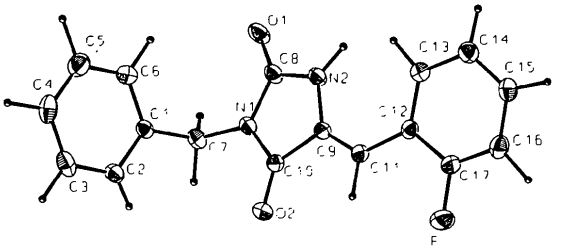


Fig. 1. Projection of $C_{17}H_{13}FN_2O_2$ showing the atom labelling with 50% probability displacement ellipsoids for non-H atoms. H atoms are of an arbitrary size.

Experimental

The synthesis of the title compound has been reported elsewhere (Amorim *et al.*, 1992).

Crystal data

$C_{17}H_{13}FN_2O_2$
M_r = 296.30
Monoclinic
$P2_1/c$
a = 13.102 (2) Å
b = 7.077 (2) Å
c = 16.233 (2) Å
β = 109.31 (2)°
V = 1420.5 (5) Å^3
Z = 4
D_x = 1.386 Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 8.25–24.00°
μ = 0.101 mm^{-1}
T = 293 (2) K
Irregular
0.45 × 0.25 × 0.15 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2618 measured reflections
2500 independent reflections
1748 observed reflections [$I > 2\sigma(I)$]
R_{int} = 0.0104
θ_{max} = 24.97°
$h = 0 \rightarrow 15$
$k = 0 \rightarrow 9$
$l = -19 \rightarrow 19$
2 standard reflections
frequency: 120 min
intensity decay: 0.7%

Refinement

Refinement on F^2
$R(F) = 0.0562$
$wR(F^2) = 0.1387$
$S = 1.110$
2500 reflections
201 parameters
H atoms riding, with one common $U = 0.085\,(3)$ Å^2
$w = 1/[\sigma^2(F_o^2) + (0.0716P)^2 + 0.5960P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.338$ e Å^{-3}
$\Delta\rho_{min} = -0.233$ e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.050 (5)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$U_{eq} = (1/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
F	0.5492 (2)	0.0574 (4)	0.10106 (12)	0.1100 (9)
O1	0.6346 (2)	−0.0005 (4)	0.57096 (13)	0.0799 (8)
O2	0.8216 (2)	0.1232 (3)	0.38575 (13)	0.0706 (6)
N1	0.7531 (2)	0.0640 (3)	0.49662 (14)	0.0522 (6)
N2	0.5782 (2)	0.0575 (3)	0.42271 (14)	0.0553 (6)
C1	0.8854 (2)	0.2551 (4)	0.6084 (2)	0.0485 (7)
C2	0.9683 (2)	0.3531 (5)	0.5941 (2)	0.0642 (8)
C3	0.9966 (3)	0.5317 (5)	0.6298 (2)	0.0777 (10)
C4	0.9420 (3)	0.6100 (5)	0.6808 (2)	0.0773 (10)
C5	0.8589 (3)	0.5118 (6)	0.6947 (2)	0.0844 (11)
C6	0.8309 (3)	0.3358 (5)	0.6587 (2)	0.0706 (9)
C7	0.8539 (2)	0.0612 (4)	0.5709 (2)	0.0582 (7)
C8	0.6524 (2)	0.0364 (4)	0.5038 (2)	0.0557 (7)
C9	0.6284 (2)	0.0928 (4)	0.3609 (2)	0.0492 (7)
C10	0.7456 (2)	0.0976 (4)	0.4114 (2)	0.0512 (7)
C11	0.5902 (2)	0.1134 (4)	0.2748 (2)	0.0522 (7)
C12	0.4797 (2)	0.1054 (4)	0.2147 (2)	0.0503 (7)
C13	0.3872 (2)	0.1248 (4)	0.2381 (2)	0.0584 (7)
C14	0.2851 (2)	0.1156 (5)	0.1769 (2)	0.0675 (8)
C15	0.2720 (3)	0.0865 (5)	0.0902 (2)	0.0681 (8)
C16	0.3614 (3)	0.0681 (5)	0.0640 (2)	0.0710 (9)
C17	0.4615 (2)	0.0771 (4)	0.1266 (2)	0.0622 (8)

Table 2. *Selected geometric parameters (Å, °)*

F—C17	1.351 (3)	N2—C8	1.362 (3)
O1—C8	1.216 (3)	N2—C9	1.392 (3)
O2—C10	1.214 (3)	C1—C7	1.503 (4)
N1—C10	1.374 (3)	C9—C11	1.327 (4)
N1—C8	1.375 (3)	C9—C10	1.483 (4)
N1—C7	1.465 (3)	C11—C12	1.455 (4)
C10—N1—C8	111.0 (2)	C11—C9—C10	122.7 (2)
C10—N1—C7	125.1 (2)	N2—C9—C10	104.8 (2)
C8—N1—C7	123.8 (2)	O2—C10—N1	125.3 (3)
C8—N2—C9	111.1 (2)	O2—C10—C9	129.1 (3)
N1—C7—C1	111.9 (2)	N1—C10—C9	105.6 (2)
O1—C8—N2	127.0 (2)	C9—C11—C12	130.3 (2)
O1—C8—N1	125.4 (3)	F—C17—C16	118.1 (3)
N2—C8—N1	107.5 (2)	F—C17—C12	117.3 (3)
C11—C9—N2	132.5 (2)	C16—C17—C12	124.6 (3)

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *CAD*-4 *Software*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ZORTEP* (Zsolnai, 1995).

This work has received partial support from FAPESP (Proc. 94/1213–5), CNPq, FAPEAL, CAPES and FINEP.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: FG1146). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1996). C**52**, 2772–2774

(*Z*)-1-(Dichloro-*p*-methoxyphenyltelluro)-1-phenyl-2-thiophenylethene

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(*Received 15 April 1996; accepted 20 June 1996*)

Abstract

The Te^{IV} atom in the title compound, $C_{21}H_{18}Cl_2OSTe$, is in a trigonal bipyramidal configuration with the lone pair of electrons occupying one of the equatorial positions. Distances and angles are: Te—Cl 2.5140 (10) and 2.5012 (10), Te—C 2.127 (3) and 2.121 (4) Å (aryl); Cl—Te—Cl 173.07 (4), Cl—Te—C 90.96 (10), 87.71 (9), 90.09 (10) and 85.36 (9), C—Te—C 99.92 (13)°.