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1-(2,6-Difluorobenzoyl)-3-[4-(trifluoromethyl)-phenyl]urea

Li Chen, Hai-Bin Song, Qing-Min Wang,* Run-Qiu Huang, Jian Shang and Chun-Hui Mao

State Key Laboratory and Institute of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, People's Republic of China

Correspondence e-mail:
cherubchenli@mail.nankai.edu.cn

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All bond lengths and anlges in the title compound, $C_{15}H_9F_5N_2O_2$, an inhibitor of chitin synthesis, are normal. The urea linkage adopts an essentially planar configuration, with an intramolecular N—H$\cdots$O hydrogen bond. Intermolecular N—H$\cdots$O hydrogen bonds link two adjacent molecules into a centrosymmetric dimer.

Key indicators

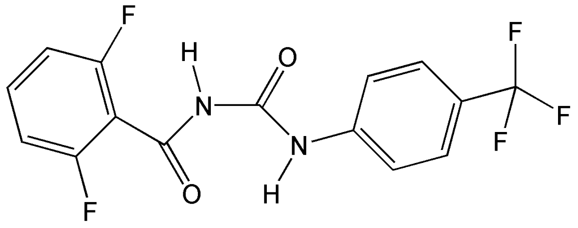
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.054
wR factor = 0.144
Data-to-parameter ratio = 10.5

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

Comment

Benzoylphenylureas, discovered in the 1970s, are known as commercial chitin formation inhibitors. In contrast to traditional pesticides, benzoylphenylurea (BPU) and its derivatives mainly control the growth and development process of insects by interfering with chitin biosynthesis and breeding (Van Daale *et al.*, 1972; Post & Vicent, 1973). Consequently, toxicity of benzoylphenylureas to vertebrates and environmental impact are very low and a high insecticidal selectivity is achieved.

Many researchers have studied the quantitative structure–activity relationship (QSAR) of BPU larvicides to analyse the effects of substituents on bioactivity (Sotomatsu *et al.*, 1987; Nakagawa *et al.*, 1988, 1991). However, owing to the fact that the actual conformation of BPUs and the structure of the acceptor are unknown, the QSAR is not clear.



(I)

In order to determine the structural character and conformation of BPUs, we have investigated the crystal structure of a well known BPU, namely 1-(2,6-difluorobenzoyl)-3-(4-trifluoromethylphenyl)urea (penfluron) (Chang & Woods, 1979) by X-ray diffraction (Fig. 1 and Table 1). The title compound, (I), contains three significant planar groupings: C1–C6 (1), N1/C8/O2/N2 (2) and C9–C14 (3). The dihedral angles between planes 1 and 2, and 2 and 3, are 43.14 (15) and 15.7 (3)°, respectively. All the atoms of the urea linkage are coplanar, thereby providing the lowest energy for the formation of an intramolecular N—H$\cdots$O hydrogen bond (Table 2), as reported (Li *et al.*, 1998; Chen *et al.*, 2004). Intermolecular N—H$\cdots$O hydrogen bonds (Table 2) link two adjacent molecules into a centrosymmetric dimer (Fig. 2).

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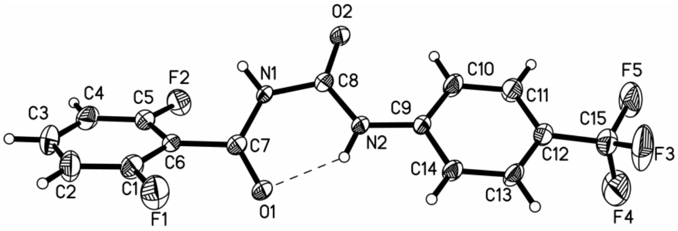

Figure 1
View of the title compound, with displacement ellipsoids drawn at the 30% probability level. The dashed line indicates an intramolecular hydrogen bond. Only the major disorder component is shown.

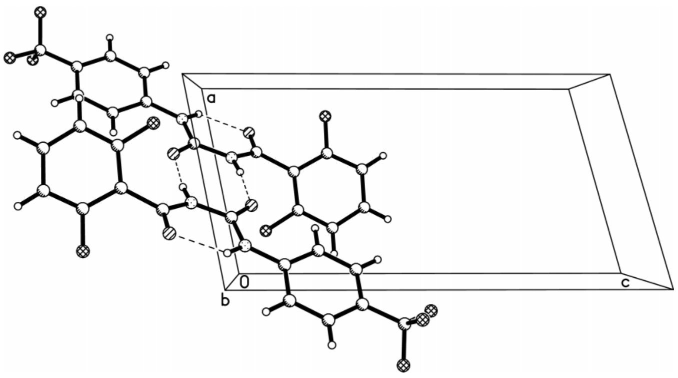

Figure 2
A partial packing diagram showing the intra- and intermolecular N—H···O hydrogen bonds (dashed lines).

Experimental

The title compound was prepared by the reaction of 4-trifluromethylaniline with 2,6-difluorobenzoyl isocyanate (Potter *et al.*, 1992). It was recrystallized from diethyl ether and gave colourless crystals.

Crystal data

$C_{15}H_9F_5N_2O_2$
$M_r = 344.24$
Triclinic, $P\bar{1}$
$a = 7.244$ (7) Å
$b = 8.014$ (8) Å
$c = 13.654$ (13) Å
$\alpha = 91.218$ (15)°
$\beta = 101.586$ (15)°
$\gamma = 108.010$ (14)°
$V = 735.5$ (12) Å^3

$Z = 2$
$D_x = 1.554$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 871 reflections
$\theta = 3.1$–24.6°
$\mu = 0.15$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.38 × 0.26 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.936$, $T_{\max} = 0.983$
3714 measured reflections

2578 independent reflections
1304 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.031$
$\theta_{\max} = 25.0°$
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -12 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.144$
$S = 1.02$
2578 reflections
245 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.003$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.229 (4)	N2—C8	1.360 (4)
O2—C8	1.227 (4)	N2—C9	1.413 (4)
N1—C7	1.362 (4)	C6—C7	1.507 (5)
N1—C8	1.402 (4)		
C7—N1—C8	129.5 (3)	O2—C8—N2	124.2 (3)
C8—N2—C9	127.6 (3)	O2—C8—N1	119.9 (3)
C5—C6—C7	123.6 (3)	N2—C8—N1	116.0 (3)
O1—C7—N1	123.6 (3)	C10—C9—N2	124.2 (3)
O1—C7—C6	120.8 (3)	C14—C9—N2	116.8 (3)
N1—C7—C6	115.6 (3)		
C8—N1—C7—O1	1.6 (6)	C9—N2—C8—O2	−1.6 (6)
C8—N1—C7—C6	−179.2 (3)	C9—N2—C8—N1	178.7 (3)
C1—C6—C7—O1	46.4 (5)	C7—N1—C8—O2	175.2 (3)
C5—C6—C7—O1	−132.6 (4)	C7—N1—C8—N2	−5.1 (5)
C1—C6—C7—N1	−132.9 (3)	C8—N2—C9—C10	−15.5 (5)
C5—C6—C7—N1	48.1 (5)	C8—N2—C9—C14	166.9 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2$^{\rm i}$	0.86	2.05	2.903 (5)	170
N2—H2A···O1	0.86	2.01	2.703 (4)	137

Symmetry code: (i) $1 - x, 1 - y, 2 - z$.

All H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and included in the final cycles of refinement using a riding model, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$, $1.2U_{\rm eq}({\rm O})$ or $1.2U_{\rm eq}({\rm N})$. The trifluoromethyl fragment is disordered between two orientations, with occupancies of 0.68 (2) and 0.32 (2), respectively.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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