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1-(2,4-Difluorophenyl)-1-[3-(2-fluorophenyl)-oxiran-2-yl]methanone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.130
Data-to-parameter ratio = 16.2

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

In the title molecule, $C_{15}H_9F_3O_2$, the bond lengths and angles are within normal ranges. The crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds.

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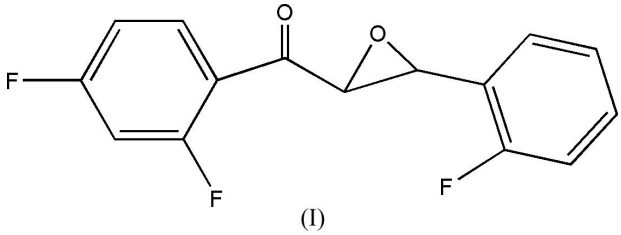
Comment

Epoxides are often used in the synthesis of organic compounds (Taylor *et al.*, 2000; Subburaj *et al.*,2002). Their ring-opening reactions (Wroblewski & Halajewska, 2002) can be used in the preparation of polyfunctional cyclic compounds. They can also be applied in stereo- and regioselective syntheses (Tan *et al.*, 2004), which could afford several diastereomeric epoxides (Subbiah *et al.*, 1999). In our search for new epoxides, the title compound, (I), has been synthesized. We report its crystal structure here.



(I)

The bond lengths and angles in (I) (Fig. 1) are within normal ranges (Table 1). The geometric parameters of the oxirane ring, C1/C2/01, are in good agreement with those found in the literature (Baures *et al.*., 1990). The mean planes *P*1 (F1/F2/C3–C9) and *P*2 (F3/C1/C10–C15) make dihedral angles of 54.71 (3) and 77.79 (2)°, respectively, with the oxirane ring.

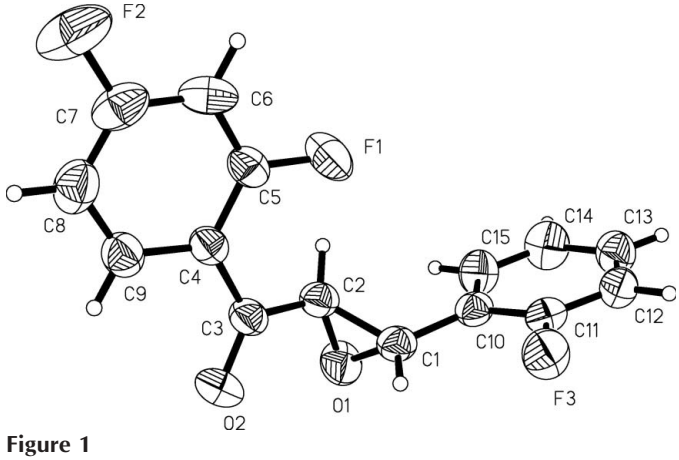


Figure 1
A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

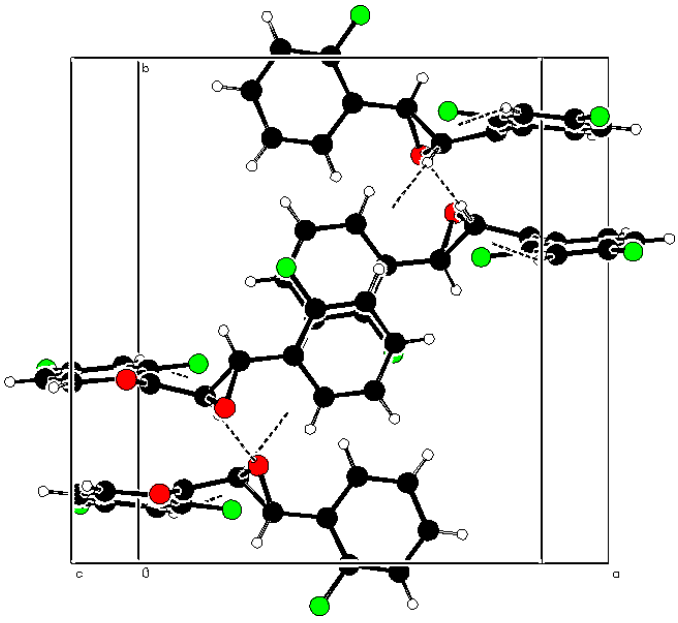


Figure 2
The packing of (I), viewed approximately along the *c* axis. Intermolecular C—H···O hydrogen bonds are shown as dashed lines.

The crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···O hydrogen bonds (Table 2).

Experimental

A mixture of 2-bromo-1-(2,4-difluorophenyl)ethanone (0.02 mol, 4.70 g), 2-fluorobenzaldehyde (0.02 mol, 2.48 g) and water (50 ml) was stirred for 1 h at room temperature. The solution was then filtered and concentrated, and the solid product was purified by recrystallization from ethanol to afford the title compound (yield 4.25 g, 85%). Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from ethyl acetate at room temperature.

Crystal data

$C_{15}H_9F_3O_2$
M_r = 278.22
Monoclinic, $P2_1/c$
a = 12.429 (2) Å
b = 13.359 (2) Å
c = 7.6176 (13) Å
β = 103.414 (2)°
V = 1230.3 (3) Å^3
Z = 4
D_x = 1.502 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1564 reflections
θ = 2.3–22.0°
μ = 0.13 mm^{-1}
T = 293 (2) K
Block, colourless
0.24 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.962, T_{max} = 0.980
8121 measured reflections
2949 independent reflections
1765 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 28.0°
$h = -16 \rightarrow 16$
$k = -10 \rightarrow 17$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.130
S = 1.05
2949 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.1661P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.011 (2)

Table 1
Selected geometric parameters (Å, °).

F1—C5	1.341 (2)	O1—C1	1.424 (2)
F2—C7	1.344 (2)	O2—C3	1.2124 (19)
F3—C11	1.358 (2)	C1—C2	1.474 (2)
O1—C2	1.418 (2)		
C2—O1—C1	62.47 (11)	O1—C2—C1	58.94 (11)
C2—C1—C10	122.48 (15)	C1—C2—C3	118.60 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.98	2.38	3.356 (2)	173
C6—H6···O2^{ii}	0.93	2.39	3.262 (2)	157

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

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.98 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, 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*.

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