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# 1-[2-(3,5-Difluorobenzyloxy)phenyl]-ethanone

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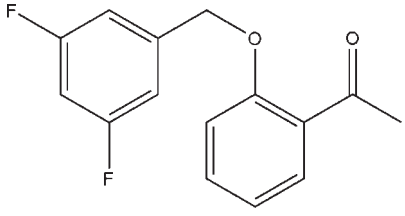
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.049; $wR$ factor = 0.153; data-to-parameter ratio = 12.9.

In the title compound, $C_{15}H_{12}F_2O_2$, the dihedral angle between the aromatic rings is 70.43 (4)°. The crystal packing exhibits no significantly short intermolecular contacts.

## Related literature

For background to the Williamson reaction in organic synthesis, see: Dermer (1934). For a related structure, see: Ma *et al.* (2010).




## Experimental

### Crystal data

$C_{15}H_{12}F_2O_2$ $M_r$ = 262.25
Triclinic, $P\overline{1}$
$a$ = 7.2808 (7) Å
$b$ = 7.9734 (8) Å
$c$ = 11.6466 (12) Å
$\alpha$ = 91.587 (1)°
$\beta$ = 106.559 (2)°
$\gamma$ = 95.343 (1)°
$V$ = 644.22 (11) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 298 K
0.42 × 0.38 × 0.20 mm

### Data collection

Bruker SMART CD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.956, $T_{max}$ = 0.979
3373 measured reflections
2239 independent reflections
1402 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.014

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.153
$S$ = 1.03
2239 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

Data collection: *SMART* (Bruker, 1996); cell refinement: *SAINT* (Bruker, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2054).

## References

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2010). E**66**, o2293 [https://doi.org/10.1107/S160053681003120X]

## 1-[2-(3,5-Difluorobenzyloxy)phenyl]ethanone

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### S1. Comment

The Williamson reaction is a very useful transformation in organic synthesis since the products are of value in both industrial and academic applications. It usually involves the reaction of an alkali-metal salt of a hydroxy compound and an alkyl halide (Dermer, 1934). In the present paper, we present the structure of the title compound, $C_{15}H_{12}F_2O_2$ (I), which was synthesized by the reaction of 1-(2-hydroxyphenyl)ethanone, potassium carbonate and 3,5-difluorobenzyl bromide. We have previously reported the structure of a compound of this type (Ma *et al.*, 2010). In (I) (Fig. 1), the ethanone group is close to coplanar with the benzene ring [torsion angle C4–C3–C2–O1, 178.8 (2)°] while the dihedral angle between the aromatic rings is 70.43 (4)°. The crystal packing exhibits no significantly short intermolecular contacts.

### S2. Experimental

1-(2-Hydroxyphenyl)ethanone (4 mmol), potassium carbonate (8 mmol), 3,5-difluorobenzyl bromide (4 mmol), and 40 ml acetone were mixed in a 100 ml flask. After 3 h stirring at 331 K, the crude product was obtained. Crystals of (I) were obtained by recrystallization from *n*-hexane/ethyl acetate.

### S3. Refinement

The positions of all H atoms were determined geometrically and refined using a riding model with C—H = 0.93–0.97 Å and $U_{iso}$(methyl H) = 1.5$U_{eq}$(C) and 1.5$U_{eq}$ for other H atoms.

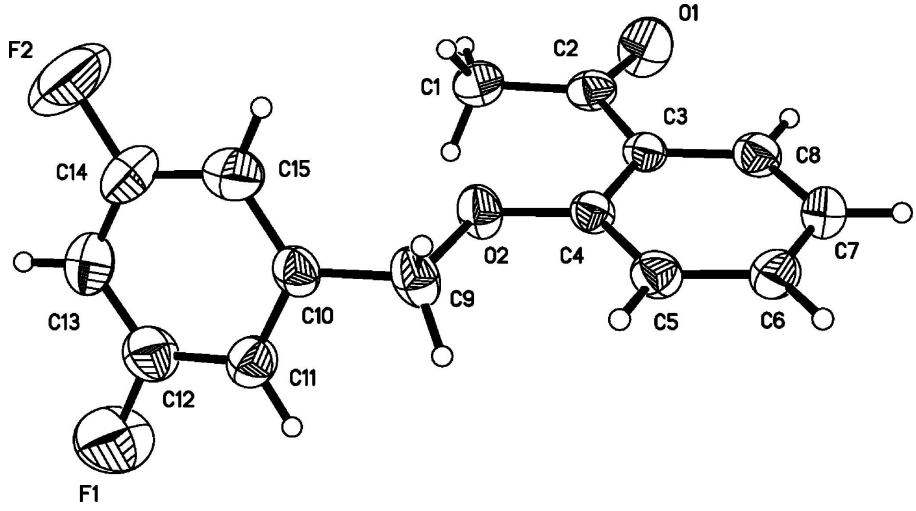


**Figure 1**

The molecular structure of (I) with atom labels, and displacement ellipsoids drawn at the 30% probability level.

## 1-[2-(3,5-Difluorobenzyloxy)phenyl]ethanone

*Crystal data*

$C_{15}H_{12}F_2O_2$
$M_r = 262.25$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.2808$ (7) Å
$b = 7.9734$ (8) Å
$c = 11.6466$ (12) Å
$\alpha = 91.587$ (1)°
$\beta = 106.559$ (2)°
$\gamma = 95.343$ (1)°
$V = 644.22$ (11) Å$^3$
$Z = 2$
$F(000) = 272$
$D_x = 1.352$ Mg m$^{-3}$
Melting point = 347–348 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1136 reflections
$\theta = 2.9$–24.8°
$\mu = 0.11$ mm$^{-1}$
$T = 298$ K
Plate, colorless
0.42 × 0.38 × 0.20 mm

*Data collection*

Bruker SMART CD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.956$, $T_{max} = 0.979$
3373 measured reflections
2239 independent reflections
1402 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 5$
$l = -13 \rightarrow 13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.153$
$S = 1.03$
2239 reflections
173 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0702P)^2 + 0.1465P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å$^{-3}$
$\Delta\rho_{min} = -0.20$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F1 | 0.1438 (3) | 0.8789 (4) | 0.0404 (2) | 0.1646 (11) |
| F2 | 0.6758 (4) | 0.6785 (4) | −0.0348 (2) | 0.1880 (13) |
| O1 | 0.7550 (3) | 0.2045 (2) | 0.54230 (18) | 0.0964 (7) |

| | | | | |
|---|---|---|---|---|
| O2 | 0.7176 (2) | 0.67975 (18) | 0.41603 (13) | 0.0629 (5) |
| C1 | 0.6631 (4) | 0.3400 (3) | 0.3629 (2) | 0.0627 (7) |
| H1A | 0.6321 | 0.2260 | 0.3292 | 0.094* |
| H1B | 0.7598 | 0.3965 | 0.3321 | 0.094* |
| H1C | 0.5495 | 0.3981 | 0.3416 | 0.094* |
| C2 | 0.7371 (3) | 0.3388 (3) | 0.4951 (2) | 0.0564 (6) |
| C3 | 0.7914 (3) | 0.4967 (3) | 0.57422 (19) | 0.0471 (5) |
| C4 | 0.7837 (3) | 0.6620 (3) | 0.53600 (19) | 0.0481 (5) |
| C5 | 0.8396 (3) | 0.7987 (3) | 0.6196 (2) | 0.0583 (6) |
| H5 | 0.8355 | 0.9080 | 0.5938 | 0.070* |
| C6 | 0.9010 (4) | 0.7728 (3) | 0.7398 (2) | 0.0659 (7) |
| H6 | 0.9379 | 0.8650 | 0.7950 | 0.079* |
| C7 | 0.9086 (4) | 0.6135 (3) | 0.7795 (2) | 0.0674 (7) |
| H7 | 0.9501 | 0.5966 | 0.8612 | 0.081* |
| C8 | 0.8540 (3) | 0.4786 (3) | 0.6971 (2) | 0.0590 (6) |
| H8 | 0.8592 | 0.3703 | 0.7247 | 0.071* |
| C9 | 0.7050 (4) | 0.8454 (3) | 0.3733 (2) | 0.0700 (7) |
| H9A | 0.8327 | 0.9048 | 0.3882 | 0.084* |
| H9B | 0.6320 | 0.9090 | 0.4138 | 0.084* |
| C10 | 0.6061 (4) | 0.8257 (3) | 0.2421 (2) | 0.0587 (6) |
| C11 | 0.4210 (4) | 0.8648 (3) | 0.1996 (2) | 0.0682 (7) |
| H11 | 0.3585 | 0.9069 | 0.2518 | 0.082* |
| C12 | 0.3289 (4) | 0.8415 (4) | 0.0801 (3) | 0.0856 (9) |
| C13 | 0.4081 (5) | 0.7794 (4) | −0.0002 (3) | 0.0902 (9) |
| H13 | 0.3405 | 0.7632 | −0.0811 | 0.108* |
| C14 | 0.5903 (6) | 0.7418 (5) | 0.0421 (3) | 0.0977 (10) |
| C15 | 0.6927 (5) | 0.7637 (4) | 0.1624 (3) | 0.0914 (9) |
| H15 | 0.8189 | 0.7365 | 0.1887 | 0.110* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F1 | 0.0955 (15) | 0.243 (3) | 0.1260 (18) | 0.0644 (17) | −0.0240 (13) | −0.0392 (17) |
| F2 | 0.187 (3) | 0.284 (4) | 0.1253 (19) | 0.063 (2) | 0.0883 (18) | −0.035 (2) |
| O1 | 0.163 (2) | 0.0435 (11) | 0.0898 (14) | 0.0206 (11) | 0.0447 (13) | 0.0108 (10) |
| O2 | 0.0905 (12) | 0.0383 (9) | 0.0520 (10) | 0.0087 (8) | 0.0073 (8) | 0.0027 (7) |
| C1 | 0.0713 (16) | 0.0452 (13) | 0.0708 (16) | 0.0032 (11) | 0.0215 (13) | −0.0080 (11) |
| C2 | 0.0622 (15) | 0.0418 (13) | 0.0717 (16) | 0.0098 (10) | 0.0285 (12) | 0.0048 (11) |
| C3 | 0.0466 (12) | 0.0453 (12) | 0.0519 (13) | 0.0099 (9) | 0.0164 (10) | 0.0051 (10) |
| C4 | 0.0481 (12) | 0.0447 (12) | 0.0507 (13) | 0.0090 (9) | 0.0117 (10) | 0.0024 (10) |
| C5 | 0.0618 (15) | 0.0463 (13) | 0.0625 (15) | 0.0097 (11) | 0.0103 (12) | −0.0028 (11) |
| C6 | 0.0668 (16) | 0.0672 (17) | 0.0589 (16) | 0.0124 (12) | 0.0101 (12) | −0.0132 (12) |
| C7 | 0.0713 (17) | 0.0807 (19) | 0.0501 (14) | 0.0160 (14) | 0.0148 (12) | 0.0049 (13) |
| C8 | 0.0598 (14) | 0.0578 (15) | 0.0646 (16) | 0.0149 (11) | 0.0227 (12) | 0.0135 (12) |
| C9 | 0.0921 (19) | 0.0431 (13) | 0.0622 (15) | 0.0051 (12) | 0.0025 (13) | 0.0081 (11) |
| C10 | 0.0715 (16) | 0.0443 (13) | 0.0597 (15) | 0.0077 (11) | 0.0166 (12) | 0.0110 (11) |
| C11 | 0.0706 (18) | 0.0718 (17) | 0.0618 (16) | 0.0081 (13) | 0.0189 (13) | −0.0016 (12) |
| C12 | 0.0740 (19) | 0.099 (2) | 0.075 (2) | 0.0192 (16) | 0.0052 (16) | −0.0020 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C13 | 0.102 (2) | 0.106 (2) | 0.0591 (18) | 0.0128 (19) | 0.0171 (17) | 0.0042 (16) |
| C14 | 0.117 (3) | 0.117 (3) | 0.076 (2) | 0.022 (2) | 0.052 (2) | −0.0050 (18) |
| C15 | 0.082 (2) | 0.105 (2) | 0.091 (2) | 0.0324 (17) | 0.0235 (17) | 0.0040 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F1—C12 | 1.359 (3) | C6—H6 | 0.9300 |
| F2—C14 | 1.340 (4) | C7—C8 | 1.372 (3) |
| O1—C2 | 1.218 (3) | C7—H7 | 0.9300 |
| O2—C4 | 1.358 (2) | C8—H8 | 0.9300 |
| O2—C9 | 1.426 (3) | C9—C10 | 1.489 (3) |
| C1—C2 | 1.480 (3) | C9—H9A | 0.9700 |
| C1—H1A | 0.9600 | C9—H9B | 0.9700 |
| C1—H1B | 0.9600 | C10—C11 | 1.365 (3) |
| C1—H1C | 0.9600 | C10—C15 | 1.368 (4) |
| C2—C3 | 1.491 (3) | C11—C12 | 1.361 (4) |
| C3—C8 | 1.389 (3) | C11—H11 | 0.9300 |
| C3—C4 | 1.404 (3) | C12—C13 | 1.336 (4) |
| C4—C5 | 1.390 (3) | C13—C14 | 1.342 (5) |
| C5—C6 | 1.371 (3) | C13—H13 | 0.9300 |
| C5—H5 | 0.9300 | C14—C15 | 1.384 (4) |
| C6—C7 | 1.365 (3) | C15—H15 | 0.9300 |
| | | | |
| C4—O2—C9 | 118.86 (17) | C7—C8—H8 | 118.6 |
| C2—C1—H1A | 109.5 | C3—C8—H8 | 118.6 |
| C2—C1—H1B | 109.5 | O2—C9—C10 | 106.94 (18) |
| H1A—C1—H1B | 109.5 | O2—C9—H9A | 110.3 |
| C2—C1—H1C | 109.5 | C10—C9—H9A | 110.3 |
| H1A—C1—H1C | 109.5 | O2—C9—H9B | 110.3 |
| H1B—C1—H1C | 109.5 | C10—C9—H9B | 110.3 |
| O1—C2—C1 | 119.4 (2) | H9A—C9—H9B | 108.6 |
| O1—C2—C3 | 118.1 (2) | C11—C10—C15 | 118.4 (2) |
| C1—C2—C3 | 122.6 (2) | C11—C10—C9 | 119.5 (2) |
| C8—C3—C4 | 116.9 (2) | C15—C10—C9 | 122.0 (3) |
| C8—C3—C2 | 117.04 (19) | C12—C11—C10 | 119.4 (3) |
| C4—C3—C2 | 126.04 (19) | C12—C11—H11 | 120.3 |
| O2—C4—C5 | 122.9 (2) | C10—C11—H11 | 120.3 |
| O2—C4—C3 | 116.96 (18) | C13—C12—F1 | 118.0 (3) |
| C5—C4—C3 | 120.2 (2) | C13—C12—C11 | 123.8 (3) |
| C6—C5—C4 | 120.2 (2) | F1—C12—C11 | 118.2 (3) |
| C6—C5—H5 | 119.9 | C12—C13—C14 | 116.5 (3) |
| C4—C5—H5 | 119.9 | C12—C13—H13 | 121.7 |
| C7—C6—C5 | 120.9 (2) | C14—C13—H13 | 121.7 |
| C7—C6—H6 | 119.6 | F2—C14—C13 | 118.8 (3) |
| C5—C6—H6 | 119.6 | F2—C14—C15 | 118.6 (4) |
| C6—C7—C8 | 118.9 (2) | C13—C14—C15 | 122.6 (3) |
| C6—C7—H7 | 120.5 | C10—C15—C14 | 119.2 (3) |
| C8—C7—H7 | 120.5 | C10—C15—H15 | 120.4 |

| | | | |
|---|---|---|---|
| C7—C8—C3 | 122.9 (2) | C14—C15—H15 | 120.4 |
| | | | |
| O1—C2—C3—C8 | −1.7 (3) | C2—C3—C8—C7 | 179.8 (2) |
| C1—C2—C3—C8 | 178.3 (2) | C4—O2—C9—C10 | −173.0 (2) |
| O1—C2—C3—C4 | 178.8 (2) | O2—C9—C10—C11 | 107.6 (3) |
| C1—C2—C3—C4 | −1.2 (3) | O2—C9—C10—C15 | −70.1 (3) |
| C9—O2—C4—C5 | 0.1 (3) | C15—C10—C11—C12 | −0.2 (4) |
| C9—O2—C4—C3 | 179.2 (2) | C9—C10—C11—C12 | −177.9 (2) |
| C8—C3—C4—O2 | −178.31 (19) | C10—C11—C12—C13 | 1.0 (5) |
| C2—C3—C4—O2 | 1.2 (3) | C10—C11—C12—F1 | 179.0 (3) |
| C8—C3—C4—C5 | 0.8 (3) | F1—C12—C13—C14 | −179.2 (3) |
| C2—C3—C4—C5 | −179.7 (2) | C11—C12—C13—C14 | −1.1 (5) |
| O2—C4—C5—C6 | 178.5 (2) | C12—C13—C14—F2 | 179.7 (3) |
| C3—C4—C5—C6 | −0.6 (3) | C12—C13—C14—C15 | 0.6 (5) |
| C4—C5—C6—C7 | 0.1 (4) | C11—C10—C15—C14 | −0.3 (4) |
| C5—C6—C7—C8 | 0.1 (4) | C9—C10—C15—C14 | 177.3 (3) |
| C6—C7—C8—C3 | 0.2 (4) | F2—C14—C15—C10 | −179.0 (3) |
| C4—C3—C8—C7 | −0.6 (3) | C13—C14—C15—C10 | 0.1 (5) |