Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(4-Benzyloxy-2-hydroxyphenyl)-ethanone

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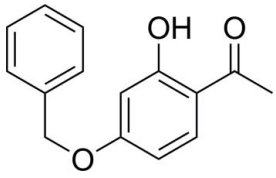
Received 11 October 2011; accepted 3 November 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.114; data-to-parameter ratio = 13.1.

The title compound, $C_{15}H_{14}O_3$, has been obtained from the reaction of 2,4-dihydroxyacetophenone, potassium carbonate and benzyl bromide. The remaining hydroxy group is involved in an intramolecular O—H···O hydrogen bond. In the crystal, intermolecular C—H···O contacts occur.

Related literature

For background to the Williamson reaction in organic synthesis, see: Dermer (1934). For synthetic procedures for related compounds, see: Mendelson *et al.* (1996). For a related structure, see: Ma *et al.* (2010).



Experimental

Crystal data

$C_{15}H_{14}O_3$
M_r = 242.26
Triclinic, $P\overline{1}$
a = 5.8433 (7) Å
b = 8.0096 (8) Å
c = 13.8089 (13) Å
α = 74.061 (1)°
β = 84.589 (1)°
γ = 87.372 (2)°
V = 618.54 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.23 × 0.20 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.987
3169 measured reflections
2167 independent reflections
1291 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.114
S = 1.02
2167 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.82	1.84	2.554 (2)	146
C1—H1B···O2^{i}	0.96	2.52	3.408 (3)	154

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 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*.

We would like to acknowledge funding support by Shaanxi Province Science and Technology (under contract No. 2011 K02–07) and the Program of Northwest A&F University (No. Z111020908).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2328).

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Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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supporting information

Acta Cryst. (2011). E**67**, o3225 [https://doi.org/10.1107/S160053681104637X]

1-(4-Benzyloxy-2-hydroxyphenyl)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 employment of an alkali-metal salt of the hydroxy compound and an alkyl halide (Dermer, 1934). Synthetic procedures to ethers derived from 2,4-dihydroxy-acetophenone as well as the structural characterisation of a related molecule have been described before (Mendelson *et al.*, 1996; Ma *et al.*, 2010).

In this paper, we present the title compound, (I), which was synthesized by the reaction of 2, 4-dihydroxy-acetone-phenone, potassium carbonate and benzyl bromide. In (I) (Fig. 1), the dihedral angle between the aromatic rings is 53.48 (4)°. The crystal packing exhibits no significantly short intermolecular contacts.

S2. Experimental

2, 4-Dihydroxy-acetonephenone (4 mmol), potassium carbonate (8 mmol), benzyl 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 (yield: 78%). Single crystals were obtained by recrystallization from methanol.

S3. Refinement

The positions of all H atoms were fixed geometrically and refined using a riding model with C—H = 0.93–0.97 Å ,O—H= 0.82 Å, and U_{iso}(H) = 1.2–1.5 U_{eq}(C, O).

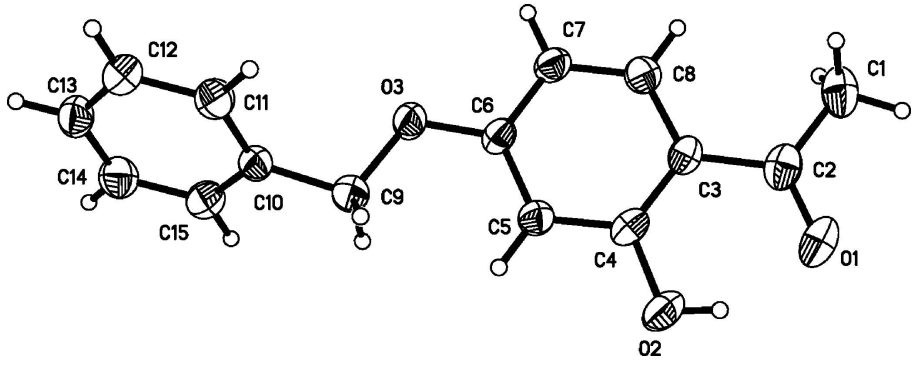

Figure 1

Molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

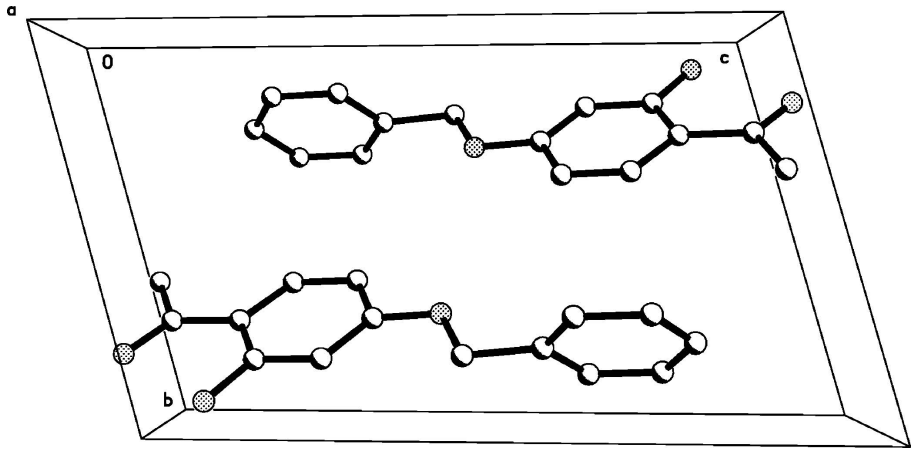

Figure 2

Crystal packing of (I) viewed along the *b* axis, with hydrogen bonds shown as dashed lines.

1-(4-Benzyloxy-2-hydroxyphenyl)ethanone

Crystal data

$C_{15}H_{14}O_3$
$M_r = 242.26$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.8433\ (7)$ Å
$b = 8.0096\ (8)$ Å
$c = 13.8089\ (13)$ Å
$\alpha = 74.061\ (1)°$
$\beta = 84.589\ (1)°$
$\gamma = 87.372\ (2)°$
$V = 618.54\ (11)$ Å^3
$Z = 2$
$F(000) = 256$
$D_x = 1.301$ Mg m^{-3}
Melting point = 378–379 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 945 reflections
$\theta = 2.7–25.4°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Triclinic, colourless
0.23 × 0.20 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.980$, $T_{max} = 0.987$
3169 measured reflections
2167 independent reflections
1291 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
$h = -6\rightarrow6$
$k = -9\rightarrow9$
$l = -16\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.114$
$S = 1.02$
2167 reflections
165 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
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ 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}
O1	0.6013 (3)	0.8182 (2)	−0.02477 (10)	0.0812 (5)
O2	0.8544 (3)	0.91909 (18)	0.08846 (10)	0.0723 (5)
H2	0.8070	0.9162	0.0349	0.108*
O3	0.6839 (2)	0.71044 (16)	0.44284 (9)	0.0584 (4)
C1	0.2766 (4)	0.6428 (3)	0.03392 (16)	0.0804 (7)
H1A	0.2655	0.6613	−0.0372	0.121*
H1B	0.1382	0.6848	0.0635	0.121*
H1C	0.2971	0.5210	0.0653	0.121*
C2	0.4770 (4)	0.7384 (3)	0.04958 (16)	0.0627 (6)
C3	0.5296 (3)	0.7344 (2)	0.15150 (13)	0.0499 (5)
C4	0.7175 (3)	0.8243 (2)	0.16617 (13)	0.0529 (5)
C5	0.7750 (3)	0.8181 (2)	0.26222 (13)	0.0520 (5)
H5	0.9021	0.8771	0.2705	0.062*
C6	0.6417 (3)	0.7236 (2)	0.34562 (13)	0.0479 (5)
C7	0.4525 (3)	0.6338 (2)	0.33393 (14)	0.0544 (5)
H7	0.3636	0.5700	0.3902	0.065*
C8	0.3993 (3)	0.6409 (2)	0.23848 (14)	0.0566 (5)
H8	0.2719	0.5815	0.2310	0.068*
C9	0.8747 (3)	0.8038 (3)	0.45748 (14)	0.0605 (6)
H9A	0.8578	0.9257	0.4220	0.073*
H9B	1.0162	0.7594	0.4301	0.073*
C10	0.8863 (3)	0.7845 (2)	0.56755 (14)	0.0501 (5)
C11	0.7172 (3)	0.8552 (3)	0.62181 (15)	0.0618 (6)
H11	0.5887	0.9088	0.5905	0.074*
C12	0.7353 (4)	0.8478 (3)	0.72185 (15)	0.0655 (6)
H12	0.6197	0.8961	0.7574	0.079*
C13	0.9239 (4)	0.7690 (3)	0.76880 (16)	0.0654 (6)
H13	0.9373	0.7646	0.8360	0.078*
C14	1.0919 (4)	0.6970 (3)	0.71643 (17)	0.0688 (6)
H14	1.2196	0.6430	0.7482	0.083*
C15	1.0730 (4)	0.7039 (3)	0.61631 (15)	0.0606 (6)
H15	1.1878	0.6535	0.5815	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1067 (13)	0.0896 (12)	0.0446 (9)	0.0045 (10)	−0.0021 (9)	−0.0160 (8)
O2	0.0836 (10)	0.0796 (11)	0.0449 (8)	−0.0142 (8)	0.0097 (7)	−0.0051 (7)
O3	0.0708 (9)	0.0625 (9)	0.0418 (8)	−0.0226 (7)	−0.0022 (6)	−0.0115 (6)
C1	0.0932 (18)	0.0912 (18)	0.0669 (15)	0.0076 (15)	−0.0257 (13)	−0.0336 (13)
C2	0.0768 (16)	0.0593 (14)	0.0544 (14)	0.0154 (12)	−0.0087 (12)	−0.0211 (11)
C3	0.0601 (13)	0.0478 (12)	0.0422 (12)	0.0036 (10)	−0.0029 (9)	−0.0139 (9)
C4	0.0627 (14)	0.0488 (12)	0.0410 (12)	0.0001 (10)	0.0065 (10)	−0.0057 (9)
C5	0.0569 (13)	0.0515 (12)	0.0464 (12)	−0.0099 (10)	−0.0014 (10)	−0.0106 (9)
C6	0.0593 (12)	0.0441 (11)	0.0385 (11)	−0.0048 (10)	0.0007 (9)	−0.0096 (9)
C7	0.0612 (13)	0.0548 (13)	0.0461 (12)	−0.0141 (10)	0.0056 (10)	−0.0134 (9)
C8	0.0581 (13)	0.0589 (13)	0.0558 (13)	−0.0075 (10)	−0.0035 (10)	−0.0202 (10)
C9	0.0640 (14)	0.0650 (14)	0.0533 (13)	−0.0178 (11)	−0.0017 (10)	−0.0158 (10)
C10	0.0537 (12)	0.0511 (12)	0.0466 (12)	−0.0088 (10)	−0.0041 (10)	−0.0137 (9)
C11	0.0546 (13)	0.0719 (15)	0.0578 (14)	0.0027 (11)	−0.0098 (10)	−0.0147 (11)
C12	0.0641 (14)	0.0770 (16)	0.0577 (14)	−0.0032 (12)	0.0022 (11)	−0.0245 (11)
C13	0.0768 (16)	0.0720 (16)	0.0485 (13)	−0.0132 (13)	−0.0077 (12)	−0.0158 (11)
C14	0.0660 (15)	0.0761 (16)	0.0606 (15)	0.0005 (12)	−0.0168 (12)	−0.0088 (12)
C15	0.0606 (14)	0.0612 (14)	0.0595 (14)	0.0012 (11)	0.0002 (11)	−0.0178 (10)

Geometric parameters (Å, º)

O1—C2	1.238 (2)	C7—H7	0.9300
O2—C4	1.347 (2)	C8—H8	0.9300
O2—H2	0.8200	C9—C10	1.493 (2)
O3—C6	1.362 (2)	C9—H9A	0.9700
O3—C9	1.430 (2)	C9—H9B	0.9700
C1—C2	1.491 (3)	C10—C15	1.377 (3)
C1—H1A	0.9600	C10—C11	1.379 (3)
C1—H1B	0.9600	C11—C12	1.380 (2)
C1—H1C	0.9600	C11—H11	0.9300
C2—C3	1.460 (3)	C12—C13	1.371 (3)
C3—C4	1.400 (3)	C12—H12	0.9300
C3—C8	1.404 (2)	C13—C14	1.365 (3)
C4—C5	1.386 (2)	C13—H13	0.9300
C5—C6	1.383 (2)	C14—C15	1.383 (3)
C5—H5	0.9300	C14—H14	0.9300
C6—C7	1.392 (2)	C15—H15	0.9300
C7—C8	1.368 (2)		
C4—O2—H2	109.5	C7—C8—H8	118.8
C6—O3—C9	117.04 (14)	C3—C8—H8	118.8
C2—C1—H1A	109.5	O3—C9—C10	109.89 (15)
C2—C1—H1B	109.5	O3—C9—H9A	109.7
H1A—C1—H1B	109.5	C10—C9—H9A	109.7
C2—C1—H1C	109.5	O3—C9—H9B	109.7

H1A—C1—H1C	109.5	C10—C9—H9B	109.7
H1B—C1—H1C	109.5	H9A—C9—H9B	108.2
O1—C2—C3	120.3 (2)	C15—C10—C11	118.14 (18)
O1—C2—C1	119.2 (2)	C15—C10—C9	120.72 (17)
C3—C2—C1	120.5 (2)	C11—C10—C9	121.03 (18)
C4—C3—C8	116.92 (17)	C10—C11—C12	121.11 (19)
C4—C3—C2	120.48 (19)	C10—C11—H11	119.4
C8—C3—C2	122.6 (2)	C12—C11—H11	119.4
O2—C4—C5	116.22 (19)	C13—C12—C11	119.94 (19)
O2—C4—C3	122.26 (17)	C13—C12—H12	120.0
C5—C4—C3	121.51 (17)	C11—C12—H12	120.0
C6—C5—C4	119.41 (19)	C14—C13—C12	119.7 (2)
C6—C5—H5	120.3	C14—C13—H13	120.2
C4—C5—H5	120.3	C12—C13—H13	120.2
O3—C6—C5	123.69 (18)	C13—C14—C15	120.3 (2)
O3—C6—C7	115.64 (16)	C13—C14—H14	119.8
C5—C6—C7	120.67 (17)	C15—C14—H14	119.8
C8—C7—C6	119.02 (18)	C10—C15—C14	120.81 (19)
C8—C7—H7	120.5	C10—C15—H15	119.6
C6—C7—H7	120.5	C14—C15—H15	119.6
C7—C8—C3	122.5 (2)		

O1—C2—C3—C4	1.6 (3)	C5—C6—C7—C8	−0.3 (3)
C1—C2—C3—C4	−179.90 (17)	C6—C7—C8—C3	0.5 (3)
O1—C2—C3—C8	−177.70 (18)	C4—C3—C8—C7	−1.0 (3)
C1—C2—C3—C8	0.8 (3)	C2—C3—C8—C7	178.29 (16)
C8—C3—C4—O2	−179.70 (16)	C6—O3—C9—C10	176.25 (14)
C2—C3—C4—O2	1.0 (3)	O3—C9—C10—C15	117.1 (2)
C8—C3—C4—C5	1.3 (3)	O3—C9—C10—C11	−66.5 (2)
C2—C3—C4—C5	−178.00 (16)	C15—C10—C11—C12	0.9 (3)
O2—C4—C5—C6	179.84 (16)	C9—C10—C11—C12	−175.56 (18)
C3—C4—C5—C6	−1.1 (3)	C10—C11—C12—C13	0.0 (3)
C9—O3—C6—C5	1.4 (2)	C11—C12—C13—C14	−0.6 (3)
C9—O3—C6—C7	−178.88 (15)	C12—C13—C14—C15	0.3 (3)
C4—C5—C6—O3	−179.73 (15)	C11—C10—C15—C14	−1.2 (3)
C4—C5—C6—C7	0.6 (3)	C9—C10—C15—C14	175.30 (19)
O3—C6—C7—C8	−179.99 (15)	C13—C14—C15—C10	0.6 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.82	1.84	2.554 (2)	146
C1—H1*B*···O2^{i}	0.96	2.52	3.408 (3)	154

Symmetry code: (i) *x*−1, *y*, *z*.