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1-(2-Hydroxy-4-isopropoxyphenyl)-2-phenylethanone

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.096
Data-to-parameter ratio = 13.9

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

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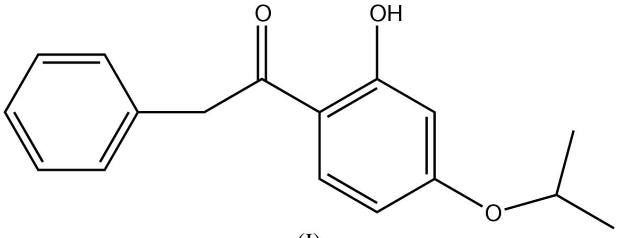
The title compound, $C_{17}H_{18}O_3$, is a product of sodium hypochlorite-induced degradation of ipriflavone, a synthetic isoflavone, which, according to some reports, is effective for prevention and treatment of postmenopausal osteoporosis. The dioxyphenyl fragment of the title molecule is almost coplanar with the carbonyl group and approximately orthogonal to the phenyl plane of the 2-phenylethanone group [the dihedral angle is 73.37 (9)°]. The molecule is stabilized by an intramolecular O—H···O bond, which closes the almost planar six-membered pseudo-ring. There is a π–π interaction between the benzene rings of hydroxyisopropoxyphenyl groups of neighbouring molecules (centroid-to-centroid distance 3.673 Å), which links the molecules into infinite chains extending along the c axis of the crystal.

Comment

Ipriflavone, a synthetic isoflavone, is currently used in several countries for prevention and treatment of involutional osteoporosis. According to some reports (Reginster, 1993), it is effective in reducing bone turnover rate, mainly through an inhibition of bone resorption. Varga *et al.* (2001) have studied its stability and chemical reactivity; they obtained the title compound, (I), $C_{17}H_{18}O_3$, by degradation of ipriflavone in basic media, using a 1 *M* solution of sodium hydroxide. We prepared the same product using the reaction of ipriflavone with sodium hypochlorite. In this paper, the crystal structure of (I) is reported.



(I)

The dioxyphenyl fragment of the hydroxyisopropoxyphenyl group in (I) (Fig. 1) is almost coplanar with the carbonyl group and approximately orthogonal to the phenyl plane of the 2-phenylethanone group [the dihedral angle is 73.37 (9)°].

The molecule of (I) is stabilized by an intramolecular O1—H1O···O2 bond (Table 2). The six-membered pseudo-ring closed by this bond is almost planar, the maximum deviation from the least-squares plane being 0.021 (9)°; it is also, in fact, coplanar with the fused C1–C6 benzene ring.

The C1–C6 benzene ring is involved in π–π stacking interactions with analogous rings of adjacent molecules, the distance between the centroids of adjacent rings being

3.673 Å. These interactions are responsible for the formation of chains, which run along the *c* axis of the crystal.

Experimental

Ipriflavone (0.5 g) was dissolved in methanol (50 ml); thereafter sodium hypochlorite (0.5 ml, 0.5% solution) was added dropwise with stirring. The mixture was refluxed for 1 h. After cooling, the mixture was poured into water (100 ml) and a colourless precipitate appeared. The precipitate was filtered and washed with water until the pH of the filtrate was 7. After recrystallization from ethanol, the product had a melting point of 351 K. Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a solution in ethanol, when the solution was left to stand for 2 d at room temperature.

Crystal data

$C_{17}H_{18}O_3$
$M_r = 270.31$
Monoclinic, $P2_1/c$
$a = 14.949\ (4)$ Å
$b = 13.366\ (2)$ Å
$c = 7.324\ (8)$ Å
$\beta = 101.214\ (8)°$
$V = 1435.5\ (16)$ Å^3
$Z = 4$

$D_x = 1.250$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1340 reflections
$\theta = 2.8$–$22.0°$
$\mu = 0.08$ mm^{-1}
$T = 298\ (2)$ K
Prism, colourless
$0.53 \times 0.28 \times 0.16$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.956$, $T_{\max} = 0.987$
7179 measured reflections

2523 independent reflections
1363 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.047$
$\theta_{\max} = 25.0°$
$h = -11 \rightarrow 17$
$k = -15 \rightarrow 15$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.096$
$S = 1.00$
2523 reflections
181 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}

Table 1
Selected torsion angles (°).

C1—C2—C7—C8	−175.8 (2)	C7—C8—C9—C14	−72.2 (3)
O2—C7—C8—C9	−10.6 (3)	C5—O3—C15—C17	−75.7 (2)
C2—C7—C8—C9	169.8 (2)	C5—O3—C15—C16	162.27 (19)
C7—C8—C9—C10	106.4 (2)		

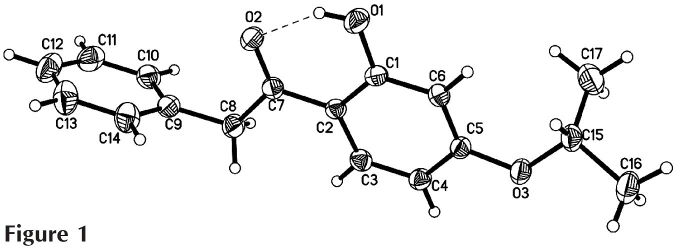


Figure 1
Molecular structure of the title compound, showing the atom numbering and 30% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···O2	0.82	1.86	2.580 (3)	146

All H atoms were placed at calculated positions and refined in riding mode, with C—H distances in the range 0.93–0.96 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ [$1.5U_{\rm eq}({\rm C})$ for methyl H atoms].

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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