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1-(2-Hydroxy-3-iodo-4,6-dimethoxyphenyl)-3-phenylprop-2-en-1-one

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The herbicide 3-phenyl-1-(2-hydroxy-3-iodo-4,6-dimethoxyphenyl)propen-1-one, $C_{17}H_{15}IO_4$, exists as a nearly planar molecule; the hydroxy group forms an intramolecular hydrogen bond with the carbonyl O atom.

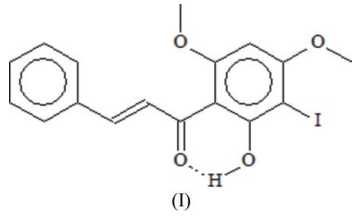
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.027
wR factor = 0.067
Data-to-parameter ratio = 17.2

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

Comment

Our earlier paper reports the structure of a propen-1-one herbicide in which the 1-carbon bears a 2-hydroxy-4,6-dimethoxyphenyl group and the 3-carbon a benzodioxol-5-yl group (Gao & Ng, 2006); the title herbicide, (I), has 2-hydroxy-3-iodo-4,6-dimethoxyphenyl and phenyl groups instead (Fig. 1). The compound adopts a similarly planar conformation and the hydroxy group also forms an intramolecular hydrogen bond with the carbonyl O atom.



(I)

Experimental

The chemical was purchased from Tianjian Bodi Chemical Reagent Company and was recrystallized from ethanol.

Crystal data

$C_{17}H_{15}IO_4$
M_r = 410.19
Orthorhombic, $Pna2_1$
a = 8.199 (2) Å
b = 14.468 (3) Å
c = 13.245 (3) Å
V = 1571.2 (5) Å^3
Z = 4
D_x = 1.734 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.05 mm^{-1}
T = 295 (2) K
Block, colorless
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.406, T_{max} = 0.684
13818 measured reflections
3522 independent reflections
3316 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 27.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.067
S = 1.10
3522 reflections
205 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2 + 0.5885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}
Absolute structure: Flack (1983), 1656 Friedel pairs
Flack parameter: 0.03 (2)

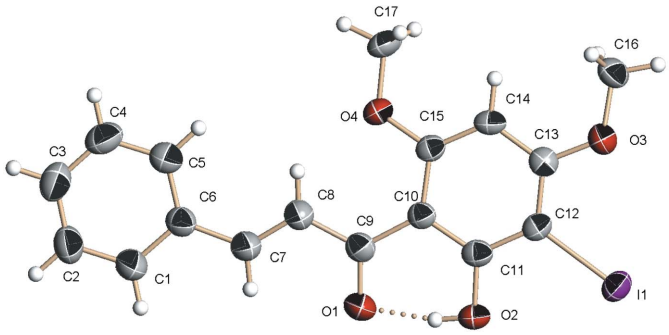


Figure 1
View of the title compound. Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii.

The carbon-bound H atoms were positionted geometrically (C—H = 0.93–0.98 Å) and were included in the refinement in the riding-model approximation, with U(H) = 1.2 or 1.5 times U_{eq}(C). The methyl groups were rotated to fit the electron density. The hydroxy H atom was located in a difference Fourier map, and was refined with a distance restraint of O—H = 0.85 (1) Å.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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