8-Hydroxy-5,6,7-trimethoxy-2-phenyl-4H-chromen-4-one

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8-Hydroxy-5,6,7-trimethoxy-2-phenyl-4H-chromen-4-one

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In the title compound, C18H16O6, the benzopyran group is essentially planar, with the O atoms of the substituent groups lying close to its mean plane. The molecular conformation is governed by intramolecular interactions. The crystal packing is mainly determined by one classical intermolecular hydrogen bond which gives rise to the formation of an infinite chain along the a axis.

Related literature
For related literature, see: Chebib & Johnston (2000); Medina et al. (1998).

Experimental

Crystal data
C18H16O6
Mr = 328.32  
Triclinic, P1  
a = 8.4536 (2) Å  
b = 9.0878 (2) Å  
c = 10.7832 (3) Å  
α = 79.545 (2)°  
β = 71.5640 (10)°  
γ = 86.925 (2)°  
V = 772.85 (3) Å³  
Z = 2

Data collection
Nonius Kappa CCD diffractometer  
Absorption correction: none  
20499 measured reflections  
3153 independent reflections  
2512 reflections with I > 2σ(I)

Refinement
R[F² > 2σ(F²)] = 0.042  
wR(F²) = 0.123  
S = 1.07  
3153 reflections  
218 parameters  
H-atom parameters constrained  
Δρ_{max} = 0.25 e Å⁻³  
Δρ_{min} = −0.24 e Å⁻³

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

D—H···A    D—H    H···A    D···A    D—H···A
O6—H8···O5  0.82    2.35    2.77 (1)  113
O6—H8···O2i 0.82    1.94    2.73 (1)  160

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

The authors are grateful to Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP) and Coordenação de Aperfeiçoamento de Pessoal de Ensino Superior (CAPES) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2176).

References
8-Hydroxy-5,6,7-trimethoxy-2-phenyl-4H-chromen-4-one

J. E. Theodoro, D. Santos, H. Pérez, M. F. das G. F. da Silva and J. Ellena

Comment

A number of different flavones are known to have interesting modulatory activities at Gamma-aminobutyric acid receptors (GABA-A), an inhibitory neurotransmitter found in the nervous systems of widely divergent species. It is the main inhibitory neurotransmitter in the central nervous system (Medina et al., 1998; Chebib & Johnston, 2000).

Figure 1 shows an ORTEP view of the title compound, 8-hydroxy-5,6,7-trimethoxy-2-phenylchromen-4-one (I) with atom labeling and 50% probability displacement ellipsoids. The benzopyran group in (I) is essentially planar, with the oxygen atoms of the substituent groups lying close to its mean plane. The ring forms angles of 113.8 (4)°, 117.8 (3)° and 114.4 (2)° with the O3—C16, O4—C17 and O5—C18 methoxy groups, respectively, and 34.61 (4)° with the phenyl ring.

The molecular conformation is fixed by intramolecular interactions (Table 1 and Figure 1). The crystal packing is mainly determined by one classical intermolecular H bond which gives rise to the formation of an infinite chain along the a axis (Table 1 and Figure 2).

Experimental

Selected parts of the Z. montana plant (Branches and leaves) were dried carefully by forced air at 40 °C and reduced to powder. The resulting material was macerated three times with hexane, followed with methanol at room temperature for 72 h each. After the evaporation of the solvent under reduced pressure, crude extracts were obtained. A well shaped single-crystal of the title compound was selected for the XRD experiments.

Refinement

All the hydrogen atoms were stereochemically positioned and refined with a riding model. Hydrogen atoms of the CH and CH2 groups were set isotropic with a thermal parameter 20% greater than the equivalent isotropic displacement parameter of the atom to which each one was bonded. This percentage was set to 50% for the hydrogen atoms of the CH3 and OH groups.

Figures

Fig. 1. View of (I) (50% probability displacement ellipsoids)
Fig. 2. View of the intermolecular interaction that gives rise to the formation of a chain along the $a$ axis.

8-Hydroxy-5,6,7-trimethoxy-2-phenyl-4H-chromen-4-one

Crystal data

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<th>Value</th>
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<td>C$<em>{18}$H$</em>{16}$O$_6$</td>
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<td>$F_{000} = 344$</td>
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<tr>
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<td>Hall symbol: -P 1</td>
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<td>$a = 8.4536$ (2) Å</td>
<td>$\lambda = 0.71073$ Å</td>
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<td>$b = 9.0878$ (2) Å</td>
<td>$\theta = 2.9\text{--}26.4^\circ$</td>
</tr>
<tr>
<td>$c = 10.7832$ (3) Å</td>
<td>$\mu = 0.11$ mm$^{-1}$</td>
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<tr>
<td>$\alpha = 79.545$ (2)$^\circ$</td>
<td>T = 294 K</td>
</tr>
<tr>
<td>$\beta = 71.5640$ (10)$^\circ$</td>
<td>Prism, yellow</td>
</tr>
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<td>$\gamma = 86.925$ (2)$^\circ$</td>
<td>$0.22 \times 0.19 \times 0.11$ mm</td>
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<td>$V = 772.85$ (3) Å$^3$</td>
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Data collection

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<td>$k = -11\rightarrow11$</td>
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<td>2512 reflections with $I &gt; 2 \sigma(I)$</td>
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Refinement

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<td>Refinement on $F^2$</td>
<td>H-atom parameters constrained</td>
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<tr>
<td>Least-squares matrix: full</td>
<td>$w = 1/[\sigma^2(F_o^2) + (0.0678P)^2 + 0.1467P]$</td>
</tr>
<tr>
<td>$R[F^2 &gt; 2\sigma(F^2)] = 0.042$</td>
<td>where $P = (F_o^2 + 2F_c^2)/3$</td>
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<tr>
<td>$wR(F^2) = 0.124$</td>
<td>$(\langle\Delta\sigma\rangle)_{\text{max}} &lt; 0.001$</td>
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<tr>
<td>$S = 1.07$</td>
<td>$\Delta\rho_{\text{max}} = 0.25$ e Å$^{-3}$</td>
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<td>$\Delta\rho_{\text{min}} = -0.24$ e Å$^{-3}$</td>
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<tr>
<td>218 parameters</td>
<td>Extinction correction: SHELXL97 (Sheldrick, 2008),</td>
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<td></td>
<td>$F_c^* = kF_c[1 + 0.001xFe^2\lambda^2/\sin(2\theta)]^{1/4}$</td>
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<tr>
<td></td>
<td>Extinction coefficient: 0.043 (11)</td>
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**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.

**Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å\(^2\))**

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supplementary materials

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Atomic displacement parameters (Å²)

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<td>C18—O5—C8—C9</td>
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Hydrogen-bond geometry (Å, °)

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Symmetry codes: (i) x+1, y, z.
Fig. 1
supplementary materials

Fig. 2