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5,7-Dimethoxy-2*H*-chromen-2-one

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Key indicators

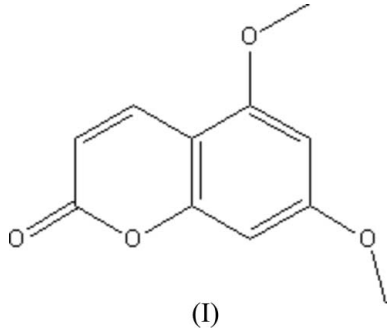
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.090
Data-to-parameter ratio = 8.5

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

The molecular structure of the title compound, $C_{11}H_{10}O_4$, contains two fused six-membered rings. All non-H atoms are constrained to be coplanar by symmetry, the molecule lying in a mirror plane.

Comment

Coumarin derivatives, found in many plants, have aromatic properties, and have been widely used as a main component for fragrances (Pang & Wang, 2005). The title compound, (I), belongs to this class of molecules. It was synthesized from 5,7-dimethoxy-2*H*-chromen-2-one (See *Experimental*) and its structure characterized (Fig. 1).



(I)

The molecular structure of (I) contains two fused six-membered rings, and all non-H atoms are coplanar, as the molecule lies on a special position, $(x, \frac{1}{4}, z)$, corresponding to a mirror plane in space group *Pnma*. The orientation of the methoxy groups is as expected, the angles with O atoms as pivots being close to 120° [C3—O3—C10 = 116.94 (17), C1—O4—C11 = 117.74 (18)°].

Experimental

The title compound was prepared according to the procedure of Pang & Wang (2005), using 5,7-dimethoxy-2*H*-chromen-2-one and dimethyl sulfate. A solution of (I) in ethanol was concentrated gradually at room temperature, to afford colourless chunks (m.p. 421–423 K).

Crystal data

$C_{11}H_{10}O_4$
M_r = 206.19
Orthorhombic, *Pnma*
a = 10.518 (3) Å
b = 6.706 (2) Å
c = 13.652 (6) Å
V = 962.9 (6) Å^3
Z = 4
D_x = 1.422 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
Chunk, colourless
0.26 × 0.21 × 0.14 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.928, T_{max} = 0.979
1021 measured reflections
938 independent reflections
704 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.2°
3 standard reflections
frequency: 60 min
intensity decay: 0.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.090
S = 1.06
938 reflections
110 parameters
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 0.1836P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.038 (6)

All H atoms were found in difference maps and refined with free coordinates and U_{iso}(H) = 0.074 Å^2. For both methyl groups C10 and C11, Fourier maps clearly indicate that one H atom lies on the mirror plane, while the others are symmetry-related in general positions.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

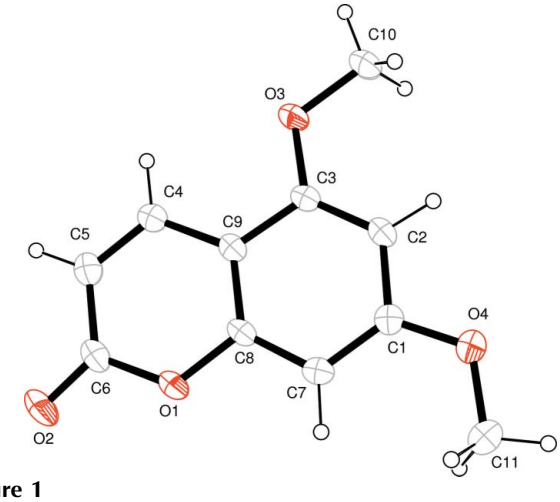


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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