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Flavone

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.108
Data-to-parameter ratio = 9.8

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

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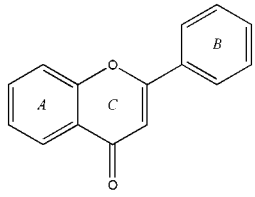
In the title molecule, $C_{15}H_{10}O_2$, there are two molecules in the asymmetric unit. The γ-pyrone ring makes a dihedral angle of 1.0 (1)° with the 2-phenyl substituent in one of the molecules, while in the other molecule the γ-pyrone ring makes a dihedral angle of 9.8 (1)° with the 2-phenyl substituent.

Comment

Flavones and related compounds are known to exhibit a wide range of interesting biological activities (Agullo *et al.*, 1997; Carlo *et al.*, 1993; Miksicek, 1993; Wang *et al.*, 1999). Flavone is the parent molecule of a number of flavones that have interesting modulatory activities at GABA-A receptors (Medina *et al.*, 1998; Chebib & Johnston, 2000). The title compound, (I), was crystallized as part of an ongoing structure–activity study to determine the properties of those compounds that confer this activity in order to aid the design of more active compounds.



(I)

All bond lengths and angles in (I) are as expected.

Experimental

The sample of flavone was obtained from Sigma–Aldrich. Single crystals of (I) were grown by slow evaporation of a methanol solution. Crystals of (I) were mounted using silicone oil which acted as both a coating and an adhesive.

Crystal data

$C_{15}H_{10}O_2$
M_r = 222.23
Orthorhombic, $P2_12_12_1$
a = 8.281 (2) Å
b = 13.216 (4) Å
c = 19.737 (6) Å
V = 2159.9 (11) Å^3
Z = 8
D_x = 1.367 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 999 reflections
θ = 1.9–28.3°
μ = 0.09 mm^{-1}
T = 150 (2) K
Block, colourless
0.40 × 0.25 × 0.25 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
14 562 measured reflections
3010 independent reflections
2762 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 28.3°
$h = -11 \rightarrow 10$
$k = -16 \rightarrow 17$
$l = -26 \rightarrow 25$

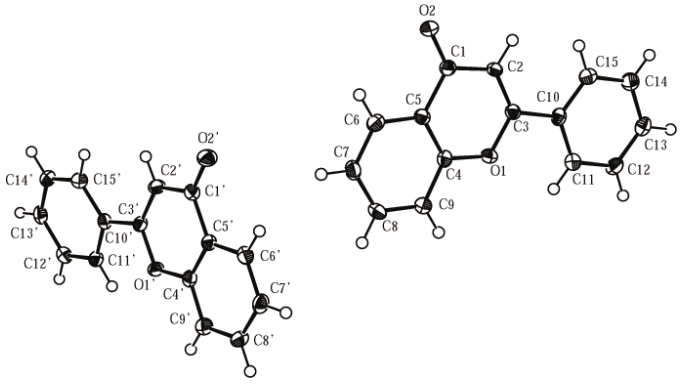


Figure 1
A general view of the asymmetric unit of (I). Ellipsoids are drawn at the 50% probability level.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2 + 0.3747P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.108$	$\Delta\rho_{max} = 0.36$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.18$ e Å^{-3}
3010 reflections	
307 parameters	
H-atom parameters constrained	

The H atoms were constrained at idealized positions.

Data collection: *SMART* (Bruker, 1995); cell refinement: *SMART* (Bruker, 1995); data reduction: *SAINT-Plus* (Bruker, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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