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Alloevodionol methyl ether

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.063
wR factor = 0.224
Data-to-parameter ratio = 14.4

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

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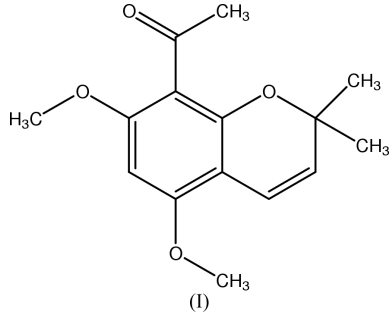
The crystal structure determination of one of the substituted α-chromene components isolated in the hexane extraction of the fruit of the indigenous Australian tree *Melicope ellyrana*, the methyl ether of the known compound alloevodionol, is reported. In this compound, 1-(5,7-dimethoxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)ethanone, $C_{15}H_{18}O_4$, the methoxy groups are approximately coplanar with the aromatic ring, while the acetyl group is normal to the ring.

Comment

The hexane-extracted components of the fruit of the indigenous Australian tree *Melicope ellyran*a (Hartley, 1981) resulted in the isolation of a number of flavonoids, and the crystal structures of two of these, *viz*. pachypodol (4′,5-dihydroxy-3,3′,7-trimethoxyflavone; Smith, Wang *et al.*, 2001) and 4′,5-dihydroxy-3,3′,8-trimethoxy-7-(3-methylbut-2-enyloxy)flavone (Smith, Bartley *et al.*, 2001), have been reported. In addition to these, several substituted α-chromenes have been isolated, including the title compound, 1-(5,7-dimethoxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl)ethanone, (I) (alloevodionol methyl ether: CA Registry No. 31367-55-2). This compound was first isolated from *Evodia elleryana* (Jones & Wright, 1946) and from *Medicosma cunninghamii*, its trivial name being given, along with the parent alloevodionol, by Sutherland (1949). It was also isolated from *Melicope simplex* (Briggs & Locker, 1950), while more recently a total of 18 variants of 2,2-dimethyl-substituted α-chromenes, including (I), were identified in the leaves of *M. ptelefolia* (Kamperdick *et al.*, 1997). Interest in the chromenes, such as (I) and its variants, has also resulted in a number of patent applications for synthetic procedures, *e.g.* Nakayama *et al.* (1979).



(I)

The crystal structure of (I) (Fig. 1) shows the 2,2-dimethyl-2*H*-1-benzopyran moiety with the methoxy substituents at C5 and C7 being close to coplanarity with the aromatic ring [torsion angles C6—C5—O5—C51 −1.8 (6)° and C6—C7—

O7—C71 −6.2 (6)°]. In contrast, the acetyl group is almost perpendicular to the ring [torsion angle C7—C8—C81—C82 94.2 (5)°]. As might be expected for this type of compound, there are no significant intermolecular associations involved in the packing in the unit cell.

Experimental

The hexane extract of the fresh fruit of *Melicope ellyrana*, after concentration (Smith, Wang *et al.*, 2001) gave a precipitate of crystals of the title compound suitable for single-crystal structural analysis.

Crystal data

$C_{15}H_{18}O_4$	D_x = 1.238 Mg m^{-3}
M_r = 262.29	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
a = 7.2233 (19) Å	θ = 12–18°
b = 10.354 (3) Å	μ = 0.09 mm^{-1}
c = 18.825 (2) Å	T = 293 (2) K
β = 91.334 (19)°	Plate, colourless
V = 1407.5 (6) Å^3	0.40 × 0.35 × 0.15 mm
Z = 4	

Data collection

Rigaku AFC-7*R* diffractometer	θ_{max} = 25.0°
ω–2θ scans	$h = 0 \rightarrow 8$
2698 measured reflections	$k = 0 \rightarrow 12$
2486 independent reflections	$l = -22 \rightarrow 22$
1106 reflections with $I > 2\sigma(I)$	3 standard reflections
R_{int} = 0.050	every 150 reflections
	intensity decay: 2.2%

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.063	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.224	$(\Delta/\sigma)_{max} < 0.001$
S = 1.39	$\Delta\rho_{max}$ = 0.32 e Å^{-3}
2486 reflections	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
173 parameters	

H atoms were included at calculated positions and were constrained in the refinement.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1999*a*); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN for Windows* (Molecular Structure Corporation, 1999*b*); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON for Windows* (Spek, 1999); software used to prepare material for publication: *TEXSAN for Windows*.

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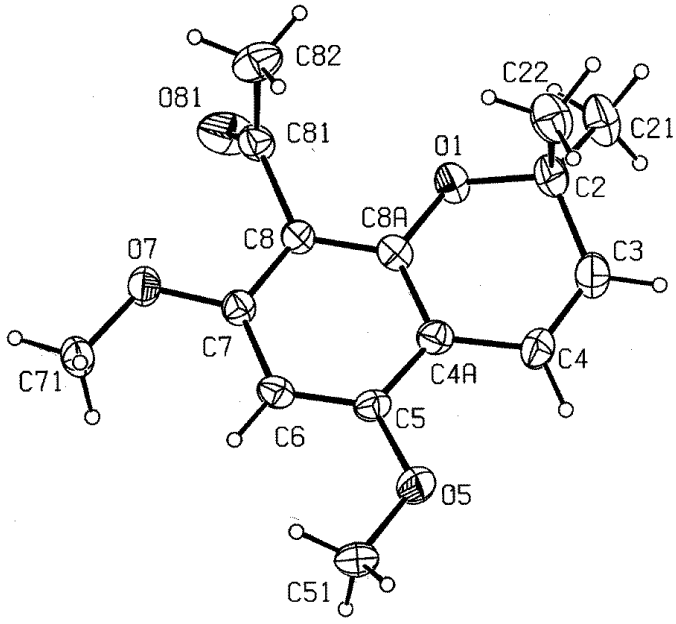

Figure 1
The molecular configuration and atom-naming scheme for the title compound. Atoms are shown as 30% probability ellipsoids (Spek, 1999).

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