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Acta Cryst. (1992). C**48**, 376–377

5-Methoxy-2-(2-methoxyphenyl)-4*H*-1-benzopyran-4-one (2,5′-Dimethoxyflavone)

BY J. C. WALLET AND E. M. GAYDOU

Laboratoire de Phytochimie, ENSSPICAM, Faculté des Sciences et des Techniques de Saint-Jêrome, Avenue Escadrille Normandie-Niemen, 13397 *Marseille CEDEX* 13, *France*

B. TINANT AND J.-P. DECLERCQ

Laboratoire de chimie physique et de cristallographie, Université Catholique de Louvain, 1 place Louis Pasteur, 1348 *Louvain-la-Neuve, Belgium*

AND A. BALDY

Faculté des Sciences et des Techniques de Saint-Jêrome, 13397 *Marseille CEDEX* 13, *France*

(*Received* 22 *April* 1991; *accepted* 11 *July* 1991)

Abstract. $C_{17}H_{14}O_4$, $M_r = 282.30$, monoclinic, $P2_1/c$, $a = 7.402$ (1), $b = 12.466$ (2), $c = 14.619$ (2) Å, $\beta = 97.25$ (1)°, $V = 1338.2$ (3) Å^3, $Z = 4$, $D_x = 1.40$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1.54178$ Å, $\mu = 8.34$ cm^{-1}, $F(000) = 592$, $T = 291$ K, $R = 0.042$ for 1684 observed reflections. The dihedral angle between the benzopyran and the phenyl ring mean planes is 10.5 (5)°.

Experimental. Crystals obtained by evaporation from ethanol. D_m not measured. Parallelepiped crystal with approximate dimensions 0.24 × 0.16 × 0.07 mm. Lattice parameters refined using 30 reflections in the range $3 \le 2\theta \le 50°$. Huber four-circle diffractometer, graphite-monochromatized Cu $K\alpha$ radiation, θ–2θ-scan technique. 2406 $hk \pm l$ measured reflections with $\sin\theta/\lambda \le 0.60$ Å^{-1}; $0 \le h \le 8$, $0 \le k \le 14$, $-17 \le l \le 16$; 1684 with $I \ge 2.5\sigma(I)$. Standard reflection ($0\bar{4}5$) checked every 50 reflections, no significant deviation. Structure solved by *SHELXS*86 (Sheldrick, 1985). H atoms from Fourier difference synthesis. Anisotropic least-squares refinement (*SHELX*76; Sheldrick, 1976) using F; H isotropic with common refined temperature factor. $w = 1/(\sigma^2 + 0.00646F^2)$, $R = 0.042$, $wR = 0.052$ for 1684 observed reflections. Final maximum shift/e.s.d. = 0.04. $S = 0.80$. Maximum and minimum heights in final difference Fourier synthesis = 0.14 and −0.20 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). The atomic parameters are given in Table 1.* Fig. 1 is a stereoscopic view of the molecule, showing the numbering of the atoms (*PLUTO*; Motherwell & Clegg, 1978). Bond distances and angles are given in Table 2.

Related literature. This work forms part of our structural investigations of methoxyflavones (Wallet, Gaydou, Tinant, Declercq, Baldy & Bonifassi, 1990; Wallet, Gaydou, Feneau-Dupont, Tinant, Declercq & Baldy, 1991). Some closely related structures have recently been described (Wallet, Gaydou, Jaud & Baldy, 1990). In 2′-methoxyflavone the torsion angle

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond lengths and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54489 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HA0073]

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Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* ($Å^2$)

$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
O1	3793 (2)	789 (1)	893 (1)	0.050 (1)
C2	4861 (3)	1490 (2)	491 (1)	0.044 (1)
C3	6680 (3)	1449 (2)	686 (1)	0.047 (1)
C4	7621 (3)	691 (2)	1327 (1)	0.046 (1)
C5	7042 (3)	−842 (2)	2417 (1)	0.045 (1)
C6	5817 (4)	−1550 (2)	2726 (2)	0.055 (1)
C7	3972 (4)	−1457 (2)	2423 (2)	0.060 (1)
C8	3302 (3)	−660 (2)	1824 (2)	0.057 (1)
C9	4555 (3)	24 (2)	1500 (1)	0.045 (1)
C10	6417 (3)	−43 (2)	1762 (1)	0.042 (1)
O11	8843 (2)	−847 (1)	2718 (1)	0.055 (1)
C12	9487 (4)	−1565 (3)	3446 (2)	0.065 (1)
O13	6203 (3)	3383 (2)	−268 (1)	0.069 (1)
C14	6989 (5)	4265 (3)	−698 (3)	0.080 (1)
O15	9287 (2)	688 (2)	1478 (1)	0.070 (1)
C1′	3728 (3)	2207 (2)	−149 (1)	0.048 (1)
C2′	4433 (4)	3128 (2)	−538 (2)	0.056 (1)
C3′	3297 (5)	3744 (2)	−1164 (2)	0.070 (1)
C4′	1492 (4)	3479 (2)	−1395 (2)	0.073 (1)
C5′	785 (4)	2597 (2)	−1000 (2)	0.069 (1)
C6′	1891 (4)	1967 (2)	−386 (2)	0.058 (1)

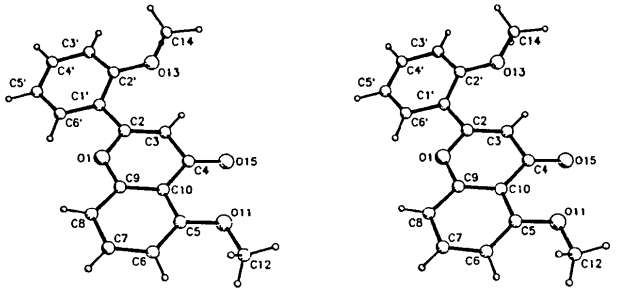

Fig. 1. Stereoscopic view of the molecule with atom numbering.

between the benzopyran and the phenyl planes is 0° while in 2′,4′,5,7-tetramethoxyflavone it is 24°. In this latter molecule a slight puckering of the benzopyran was observed; in the title compound all the endocyclic torsion angles have values less than 3 (1)° and the maximum deviation from the best mean plane through the ten atoms of the heterocycle is 0.05 (1) Å.

Table 2. *Bond distances* (Å) *and bond angles* (°)

C2—O1	1.360 (3)	C9—O1	1.374 (2)
C3—C2	1.341 (3)	C1′—C2	1.477 (3)
C4—C3	1.447 (3)	C10—C4	1.476 (3)
O15—C4	1.225 (3)	C6—C5	1.382 (3)
C10—C5	1.417 (3)	O11—C5	1.351 (3)
C7—C6	1.387 (4)	C8—C7	1.375 (3)
C9—C8	1.387 (3)	C10—C9	1.386 (3)
C12—O11	1.426 (3)	C14—O13	1.426 (3)
C2′—O13	1.357 (3)	C2′—C1′	1.410 (3)
C6′—C1′	1.392 (3)	C3′—C2′	1.393 (3)
C4′—C3′	1.377 (4)	C5′—C4′	1.375 (4)
C6′—C5′	1.381 (3)		

C9—O1—C2	120.7 (2)	C3—C2—O1	120.5 (2)
C1′—C2—O1	110.3 (2)	C1′—C2—C3	129.2 (2)
C4—C3—C2	123.4 (2)	C10—C4—C3	114.6 (2)
O15—C4—C3	120.7 (2)	O15—C4—C10	124.7 (2)
C10—C5—C6	119.9 (2)	O11—C5—C6	123.5 (2)
O11—C5—C10	116.6 (2)	C7—C6—C5	120.1 (2)
C8—C7—C6	121.7 (2)	C9—C8—C7	117.3 (2)
C8—C9—O1	114.2 (2)	C10—C9—O1	122.2 (2)
C10—C9—C8	123.6 (2)	C5—C10—C4	124.3 (2)
C9—C10—C4	118.5 (2)	C9—C10—C5	117.2 (2)
C12—O11—C5	118.0 (2)	C2′—O13—C14	119.0 (2)
C2′—C1′—C2	122.6 (2)	C6′—C1′—C2	119.1 (2)
C6′—C1′—C2′	118.3 (2)	C1′—C2′—O13	117.8 (2)
C3′—C2′—O13	122.8 (2)	C3′—C2′—C1′	119.3 (3)
C4′—C3′—C2′	121.0 (3)	C5′—C4′—C3′	119.9 (2)
C6′—C5′—C4′	120.1 (3)	C5′—C6′—C1′	121.3 (3)

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Acta Cryst. (1992). C**48**, 377–379

5-Hydroxy-5-methylsydno[3,4-*a*]indole

BY DAVID A. GROSSIE AND K. TURNBULL

Department of Chemistry, Wright State University, Dayton, Ohio 45435, *USA*

(*Received* 20 *May* 1991; *accepted* 24 *July* 1991)

Abstract. $C_{10}H_8N_2O_3$, $M_r = 204.18$, monoclinic, $P2_1/a$, $a = 8.702$ (4), $b = 12.063$ (2), $c = 9.711$ (4) Å, $\beta = 115.10$ (2)°, $V = 923.1$ (6) Å^3, $Z = 4$, $D_x = 1.47$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 1.04$ cm^{-1}, $F(000) = 424$, $T = 296$ K, final $R = 0.047$ for 1843 reflections with $I > 3\sigma(I)$. The sydnone ring exhibits

0108-2701/92/020377-03$03.00