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5,7-Dimethoxy-3-(4-methoxyphenyl)-4*H*-chromen-4-one

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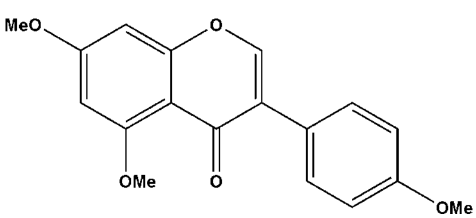
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.145; data-to-parameter ratio = 13.5.

In the genistein-related title molecule, $C_{18}H_{16}O_5$, the dihedral angle between the two benzene rings is 59.25 (6)°.

Related literature

For reference structural data, see: Allen *et al.* (1987). For background, see: Kim *et al.* (2004); Li *et al.* (2006).



Experimental

Crystal data

$C_{18}H_{16}O_5$
M_r = 312.31
Triclinic, $P\bar{1}$
a = 8.5649 (10) Å
b = 10.3212 (13) Å
c = 10.5563 (13) Å
α = 63.783 (2)°
β = 71.937 (2)°
γ = 65.953 (2)°
V = 754.83 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
0.20 × 0.15 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001) T_{min} = 0.980, T_{max} = 0.985
4140 measured reflections
2855 independent reflections
2134 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.145
S = 1.03
2855 reflections
211 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2521).

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supplementary materials

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5,7-Dimethoxy-3-(4-methoxyphenyl)-4*H*-chromen-4-one

H.-Q. Li, Z.-P. Xiao, Y. Han, R.-Q. Fang and H.-L. Zhu

Comment

Genistein derivatives show various biological activitites (Kim *et al.*, 2004; Li *et al.*, 2006). In the genistein-related title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the least-squares planes of the two benzene rings (C2—C7 and C1—C15) is 59.25 (6) °. The crystal packing is stabilized by van der Waals forces.

Experimental

Genistein (0.41 g, 1.5 mmol), iodomethane (0.62 ml, 6 mmol) and potassium carbonate (0.14 g, 1 mmol) in 50 ml of dry acetone were sonicated. After the completion of reaction, the mixture was cooled to room temperature and filtered. The filtrate was distilled to give a yellow solid, which was washed with aqueous saturated sodium bicarbonate twice. The solid was dissolved in acetone (15 ml) and stirred for about 10 min to give a clear solution. After keeping the solution in air for 10 d, colourless blocks of (I) were formed at the bottom of the vesssl on slow evaporation of the solvent. They were collected, washed three times with acetone and dried in a vacuum desiccator using $CaCl_2$ (yield = 88%).

Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

Figures

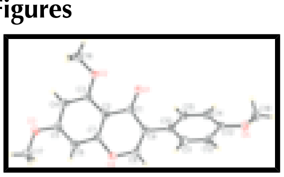


Fig. 1. The molecular structure of (I) showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms).

5,7-Dimethoxy-3-(4-methoxyphenyl)-4*H*-chromen-4-one

Crystal data

$C_{18}H_{16}O_5$	$Z = 2$
$M_r = 312.31$	$F_{000} = 328$
Triclinic, $P\overline{1}$	$D_x = 1.374$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 8.5649$ (10) Å	Cell parameters from 1220 reflections

b = 10.3212 (13) Å	θ = 2.5–25.5°
c = 10.5563 (13) Å	μ = 0.10 mm^{-1}
α = 63.783 (2)°	T = 298 (2) K
β = 71.937 (2)°	Block, colorless
γ = 65.953 (2)°	0.20 × 0.15 × 0.15 mm
V = 754.83 (16) Å^3	

Data collection

Bruker SMART CCD diffractometer	2855 independent reflections
Radiation source: fine-focus sealed tube	2134 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.016
T = 298(2) K	θ_{max} = 26.0°
ω scans	θ_{min} = 2.2°
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -8 \rightarrow 10$
T_{min} = 0.980, T_{max} = 0.985	$k = -12 \rightarrow 12$
4140 measured reflections	$l = -13 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H-atom parameters constrained
$wR(F^2)$ = 0.145	$w = 1/[\sigma^2(F_o^2) + (0.0767P)^2 + 0.0778P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
2855 reflections	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
211 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.4469 (2)	0.3920 (2)	0.7581 (2)	0.0375 (5)
C2	0.4112 (2)	0.2474 (2)	0.8110 (2)	0.0338 (4)
C3	0.2547 (2)	0.2205 (2)	0.8986 (2)	0.0365 (5)
C4	0.2282 (2)	0.0844 (2)	0.9375 (2)	0.0408 (5)
H4	0.1239	0.0702	0.9921	0.049*
C5	0.3565 (3)	−0.0329 (2)	0.8960 (2)	0.0389 (5)
C6	0.5120 (3)	−0.0150 (2)	0.8167 (2)	0.0411 (5)
H6	0.5987	−0.0931	0.7900	0.049*
C7	0.5355 (2)	0.1237 (2)	0.7778 (2)	0.0359 (4)
C8	0.7358 (3)	0.2583 (2)	0.6647 (2)	0.0485 (6)
H8	0.8475	0.2585	0.6183	0.058*
C9	0.6278 (2)	0.3838 (2)	0.6895 (2)	0.0381 (5)
C10	0.6923 (2)	0.5133 (2)	0.6466 (2)	0.0376 (5)
C11	0.8407 (3)	0.4916 (2)	0.6911 (2)	0.0493 (5)
H11	0.8984	0.3953	0.7502	0.059*
C12	0.9041 (3)	0.6105 (2)	0.6491 (3)	0.0497 (6)
H12	1.0027	0.5941	0.6810	0.060*
C13	0.8212 (2)	0.7534 (2)	0.5600 (2)	0.0393 (5)
C14	0.6747 (2)	0.7777 (2)	0.5130 (2)	0.0431 (5)
H14	0.6192	0.8736	0.4517	0.052*
C15	0.6110 (2)	0.6575 (2)	0.5581 (2)	0.0422 (5)
H15	0.5108	0.6748	0.5278	0.051*
C16	−0.0023 (3)	0.3017 (3)	1.0530 (3)	0.0615 (7)
H16A	−0.0738	0.2767	1.0187	0.092*
H16B	−0.0698	0.3891	1.0792	0.092*
H16C	0.0419	0.2170	1.1350	0.092*
C17	0.4422 (3)	−0.2884 (2)	0.9073 (3)	0.0600 (6)
H17A	0.4685	−0.2596	0.8052	0.090*
H17B	0.3976	−0.3725	0.9482	0.090*
H17C	0.5455	−0.3178	0.9445	0.090*
C18	0.8265 (3)	1.0087 (3)	0.4181 (3)	0.0612 (7)
H18A	0.8342	0.9953	0.3318	0.092*
H18B	0.8923	1.0733	0.3992	0.092*
H18C	0.7076	1.0548	0.4520	0.092*
O1	0.33992 (18)	0.51091 (16)	0.76789 (19)	0.0600 (5)
O2	0.13918 (17)	0.33485 (15)	0.94267 (16)	0.0493 (4)
O3	0.31532 (18)	−0.16221 (15)	0.94307 (17)	0.0519 (4)
O4	0.69615 (17)	0.13026 (15)	0.70162 (17)	0.0510 (4)
O5	0.89364 (17)	0.86501 (16)	0.52360 (17)	0.0500 (4)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0365 (10)	0.0374 (11)	0.0389 (11)	−0.0124 (9)	0.0012 (8)	−0.0184 (9)

C2	0.0336 (10)	0.0345 (10)	0.0344 (10)	−0.0110 (8)	−0.0029 (8)	−0.0150 (8)
C3	0.0348 (10)	0.0345 (10)	0.0413 (11)	−0.0104 (8)	−0.0028 (8)	−0.0175 (8)
C4	0.0365 (11)	0.0416 (11)	0.0472 (12)	−0.0169 (9)	−0.0002 (9)	−0.0186 (9)
C5	0.0462 (11)	0.0334 (10)	0.0402 (11)	−0.0154 (9)	−0.0079 (9)	−0.0128 (9)
C6	0.0444 (12)	0.0330 (10)	0.0446 (12)	−0.0072 (9)	−0.0060 (9)	−0.0183 (9)
C7	0.0349 (10)	0.0359 (10)	0.0353 (10)	−0.0110 (8)	−0.0012 (8)	−0.0146 (8)
C8	0.0367 (11)	0.0445 (12)	0.0607 (14)	−0.0183 (9)	0.0093 (10)	−0.0223 (11)
C9	0.0361 (10)	0.0395 (11)	0.0377 (11)	−0.0145 (8)	−0.0006 (8)	−0.0145 (9)
C10	0.0329 (10)	0.0422 (11)	0.0377 (11)	−0.0148 (8)	0.0024 (8)	−0.0171 (9)
C11	0.0435 (12)	0.0431 (12)	0.0543 (13)	−0.0127 (9)	−0.0129 (10)	−0.0092 (10)
C12	0.0380 (11)	0.0512 (13)	0.0626 (14)	−0.0154 (10)	−0.0136 (10)	−0.0180 (11)
C13	0.0331 (10)	0.0434 (11)	0.0434 (11)	−0.0174 (9)	0.0033 (8)	−0.0188 (9)
C14	0.0380 (11)	0.0407 (11)	0.0451 (12)	−0.0137 (9)	−0.0067 (9)	−0.0099 (9)
C15	0.0345 (10)	0.0483 (12)	0.0445 (12)	−0.0159 (9)	−0.0065 (9)	−0.0149 (10)
C16	0.0504 (13)	0.0597 (15)	0.0775 (17)	−0.0275 (11)	0.0240 (12)	−0.0411 (13)
C17	0.0688 (16)	0.0355 (12)	0.0774 (17)	−0.0156 (11)	−0.0080 (13)	−0.0253 (12)
C18	0.0598 (14)	0.0489 (13)	0.0766 (18)	−0.0280 (11)	−0.0104 (13)	−0.0148 (12)
O1	0.0452 (9)	0.0401 (8)	0.0895 (13)	−0.0177 (7)	0.0184 (8)	−0.0344 (8)
O2	0.0397 (8)	0.0420 (8)	0.0658 (10)	−0.0188 (6)	0.0165 (7)	−0.0305 (7)
O3	0.0555 (9)	0.0361 (8)	0.0683 (10)	−0.0195 (7)	−0.0031 (7)	−0.0225 (7)
O4	0.0408 (8)	0.0418 (8)	0.0638 (10)	−0.0142 (6)	0.0141 (7)	−0.0275 (7)
O5	0.0423 (8)	0.0452 (8)	0.0665 (10)	−0.0205 (7)	−0.0061 (7)	−0.0194 (8)

Geometric parameters (Å, °)

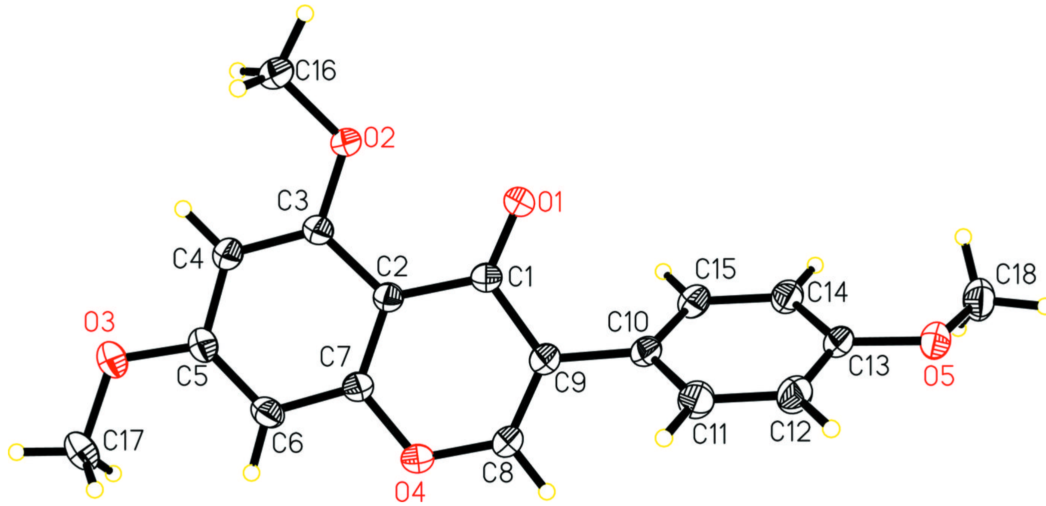
C1—O1	1.222 (2)	C11—H11	0.9300
C1—C2	1.471 (3)	C12—C13	1.378 (3)
C1—C9	1.478 (3)	C12—H12	0.9300
C2—C7	1.393 (2)	C13—O5	1.379 (2)
C2—C3	1.427 (3)	C13—C14	1.380 (3)
C3—O2	1.355 (2)	C14—C15	1.390 (3)
C3—C4	1.373 (3)	C14—H14	0.9300
C4—C5	1.397 (3)	C15—H15	0.9300
C4—H4	0.9300	C16—O2	1.433 (3)
C5—O3	1.357 (2)	C16—H16A	0.9600
C5—C6	1.372 (3)	C16—H16B	0.9600
C6—C7	1.386 (3)	C16—H16C	0.9600
C6—H6	0.9300	C17—O3	1.430 (2)
C7—O4	1.374 (2)	C17—H17A	0.9600
C8—C9	1.332 (3)	C17—H17B	0.9600
C8—O4	1.358 (2)	C17—H17C	0.9600
C8—H8	0.9300	C18—O5	1.419 (3)
C9—C10	1.486 (3)	C18—H18A	0.9600
C10—C15	1.380 (3)	C18—H18B	0.9600
C10—C11	1.390 (3)	C18—H18C	0.9600
C11—C12	1.382 (3)		
O1—C1—C2	124.71 (17)	C13—C12—H12	120.0
O1—C1—C9	121.14 (18)	C11—C12—H12	120.0
C2—C1—C9	114.15 (15)	C12—C13—O5	116.05 (17)

C7—C2—C3	115.23 (17)	C12—C13—C14	119.94 (18)
C7—C2—C1	120.16 (17)	O5—C13—C14	124.01 (18)
C3—C2—C1	124.60 (16)	C13—C14—C15	119.33 (18)
O2—C3—C4	123.17 (18)	C13—C14—H14	120.3
O2—C3—C2	115.90 (16)	C15—C14—H14	120.3
C4—C3—C2	120.91 (17)	C10—C15—C14	121.74 (18)
C3—C4—C5	120.67 (18)	C10—C15—H15	119.1
C3—C4—H4	119.7	C14—C15—H15	119.1
C5—C4—H4	119.7	O2—C16—H16A	109.5
O3—C5—C6	124.45 (17)	O2—C16—H16B	109.5
O3—C5—C4	114.90 (18)	H16A—C16—H16B	109.5
C6—C5—C4	120.63 (18)	O2—C16—H16C	109.5
C5—C6—C7	117.72 (17)	H16A—C16—H16C	109.5
C5—C6—H6	121.1	H16B—C16—H16C	109.5
C7—C6—H6	121.1	O3—C17—H17A	109.5
O4—C7—C6	113.70 (16)	O3—C17—H17B	109.5
O4—C7—C2	121.58 (17)	H17A—C17—H17B	109.5
C6—C7—C2	124.72 (18)	O3—C17—H17C	109.5
C9—C8—O4	125.33 (18)	H17A—C17—H17C	109.5
C9—C8—H8	117.3	H17B—C17—H17C	109.5
O4—C8—H8	117.3	O5—C18—H18A	109.5
C8—C9—C1	119.66 (18)	O5—C18—H18B	109.5
C8—C9—C10	118.99 (17)	H18A—C18—H18B	109.5
C1—C9—C10	121.35 (16)	O5—C18—H18C	109.5
C15—C10—C11	117.72 (18)	H18A—C18—H18C	109.5
C15—C10—C9	121.51 (17)	H18B—C18—H18C	109.5
C11—C10—C9	120.74 (18)	C3—O2—C16	117.51 (16)
C12—C11—C10	121.22 (19)	C5—O3—C17	117.94 (17)
C12—C11—H11	119.4	C8—O4—C7	118.44 (14)
C10—C11—H11	119.4	C13—O5—C18	118.07 (16)
C13—C12—C11	120.04 (19)		

O1—C1—C2—C7	171.3 (2)	C2—C1—C9—C10	−172.17 (16)
C9—C1—C2—C7	−8.5 (3)	C8—C9—C10—C15	124.8 (2)
O1—C1—C2—C3	−9.5 (3)	C1—C9—C10—C15	−54.9 (3)
C9—C1—C2—C3	170.60 (17)	C8—C9—C10—C11	−53.1 (3)
C7—C2—C3—O2	174.17 (16)	C1—C9—C10—C11	127.1 (2)
C1—C2—C3—O2	−5.0 (3)	C15—C10—C11—C12	0.5 (3)
C7—C2—C3—C4	−4.1 (3)	C9—C10—C11—C12	178.5 (2)
C1—C2—C3—C4	176.71 (18)	C10—C11—C12—C13	−0.8 (3)
O2—C3—C4—C5	−176.06 (18)	C11—C12—C13—O5	−179.94 (19)
C2—C3—C4—C5	2.1 (3)	C11—C12—C13—C14	0.1 (3)
C3—C4—C5—O3	179.07 (17)	C12—C13—C14—C15	0.9 (3)
C3—C4—C5—C6	0.6 (3)	O5—C13—C14—C15	−179.00 (18)
O3—C5—C6—C7	−179.33 (18)	C11—C10—C15—C14	0.6 (3)
C4—C5—C6—C7	−1.0 (3)	C9—C10—C15—C14	−177.37 (18)
C5—C6—C7—O4	178.55 (17)	C13—C14—C15—C10	−1.3 (3)
C5—C6—C7—C2	−1.3 (3)	C4—C3—O2—C16	10.6 (3)
C3—C2—C7—O4	−176.04 (16)	C2—C3—O2—C16	−167.67 (19)
C1—C2—C7—O4	3.2 (3)	C6—C5—O3—C17	−0.2 (3)

C3—C2—C7—C6	3.8 (3)	C4—C5—O3—C17	−178.62 (18)
C1—C2—C7—C6	−176.97 (17)	C9—C8—O4—C7	−3.9 (3)
O4—C8—C9—C1	−2.2 (3)	C6—C7—O4—C8	−176.59 (18)
O4—C8—C9—C10	178.07 (19)	C2—C7—O4—C8	3.3 (3)
O1—C1—C9—C8	−171.8 (2)	C12—C13—O5—C18	172.12 (19)
C2—C1—C9—C8	8.1 (3)	C14—C13—O5—C18	−7.9 (3)
O1—C1—C9—C10	8.0 (3)		

Fig. 1


C16
O2
O1
C3
C4
C2
C1
C15
C14
C18
O3
C5
C7
C10
C13
O5
C9
C6
C11
C12
C17
C8
O4