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3-(3-Methoxybenzylidene)chroman-4-one

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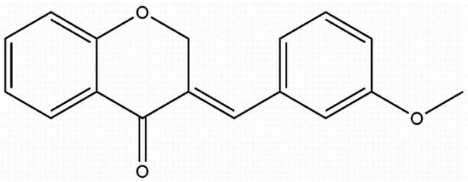
Key indicators: single-crystal X-ray study; T = 446 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.112; data-to-parameter ratio = 12.7.

In the title compound, $C_{17}H_{14}O_3$, the dihedral angle between the methoxybenzene unit and the benzene ring of the chromanone system is 64.12 (3)°. The crystal structure is stabilized by weak C—H⋯O interactions.

Related literature

For the preparation, see: Shaikh *et al.* (2011). For related structures, see: Kirkiacharian *et al.* (1984); Marx *et al.* (2008); Suresh *et al.* (2007); Chantrapromma *et al.* (2006); Augustine *et al.* (2008). For the biological activity of this class of compound, see: du Toit *et al.* (2010).



Experimental

Crystal data

$C_{17}H_{14}O_3$
M_r = 266.28
Monoclinic, $P2_1/c$
a = 12.4143 (9) Å
b = 6.7141 (5) Å
c = 16.0031 (10) Å
β = 98.658 (4)°
V = 1318.67 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 446 K
0.28 × 0.21 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
4414 measured reflections
2315 independent reflections
1662 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.00
2315 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.21 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.20 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C2—H2B⋯O1$^{\rm i}$	0.97	2.54	3.3808 (19)	145
C18—H18B⋯O3$^{\rm ii}$	0.96	2.50	3.4227 (19)	161

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We thank the University of KwaZulu-Natal, the National Research Foundation (NRF) and the South African Research Chairs initiative of the Department of Science and Technology for financial support and Ms Hong Su for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2528).

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supplementary materials

Acta Cryst. (2012). E**68**, o1006   [doi:10.1107/S160053681200949X]

3-(3-Methoxybenzylidene)chroman-4-one

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Comment

The title compound, 3-(3-Methoxybenzylidene)-chroman-4-one, belongs to a class of compounds called homoisoflavonoids, which are C-16, *α*,*β* unsaturated carbonyl compounds containing two aromatic rings. They are a group of naturally occurring molecules that are structurally related to isoflavonoids but differ by containing one more carbon atom (Kirkiacharian *et al.*, 1984). Homoisoflavonoids may be categorized into four groups depending on the type of structural backbone present. The four groups are 3-benzylidene-4-chromanones, of which the title compound belongs to as well as the 3-benzyl-4-chromanones, 3-benzyl-3-hydroxy-4-chromanones and scillascillins (du Toit *et al.*, 2010).

This compound may undergo chemical conversion into the (E)- and (*Z*)-isomers (Kirkiacharian *et al.*, 1984). The 3-benzylidene-4-chromanones have been shown to display a wide range of biological activities (du Toit *et al.*, 2010). The most commonly used procedure for the synthesis of homoisoflavoinoids involves the condensation of chroman-4-one with an aromatic aldehyde in the presence of an acidic or basic catalyst (Shaikh *et al.*, 2011).

In the molecular structure, the dihedral angle between the methoxybenzene moeity and the benzene ring of the chromanone moiety is 64.12 (3) °.The Chromanone moiety is fused with a phenyl ring and adopts a half chair conformation (Fig 1). The molecule of (I) is stablized by two weak C—H···O intramolecular interactions (Table 1).

Experimental

A mixture of chroman-4-one (1 g, 6.749 mmol), 3-methoxybenzaldehyde (1.103 g, 8.099 mmol) and 10–15 drops of piperidine was heated at 80°C for 20 hrs. The reaction mixture was monitored for completion by thin layer chromatography. Upon completion, the reaction mixture was cooled, diluted with water and neutralized using 10% HCl. The reaction mixture was extracted with ethyl acetate (3 × 30 mL). The ethyl acetate layers were combined, washed with brine (20 ml), water (2 × 10 mL) and dried over anhydrous magnesium sulfate. The solvent was reduced and the compound purified by column chromatography using silica gel (Merck 9385, 40–63 μm particle size) with a mobile phase of 2% ethyl acetate in hexane to yield the title compound with a m.p. of 85–86°C.

^{1}H NMR: δ (ppm): 3.83 (3*H*, s, OCH_3), 5.36 (2*H*, d, *J* = 1.72 Hz, 2*H*-2), 6.82 (1*H*, s, H-2′), 6.87 (1*H*, d, *J* = 7.60 Hz, H-6′), 6.93 (2*H*, m, H-8, H-4′), 7.05 (1*H*, t, *J* = 7.52 Hz, H-6), 7.34 (1*H*, t, *J* = 7.92 Hz, H-5′), 7.47 (1*H*, t, *J* = 8.52 Hz, H-7), 7.82 (1*H*, s, H-9), 8.00 (1*H*, dd, *J* = 7.82, 1.46 Hz, H-5). ^{13}C NMR: δ (ppm): 55.36 (OCH_3), 67.66 (C-2), 115.06 (C-4′), 115.42 (C-2′), 117.93 (C-8), 121.92 (C-6), 122.02 (C-4a), 122.28 (C-6′), 127.96 (C-5), 129.76 (C-5′), 131.15 (C-3), 135.69 (C-1′), 135.90 (C-7), 137.40 (C-9), 159.69 (C-3′), 161.18 (C-8a), 182.23(C-4).

Computing details

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008);

program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

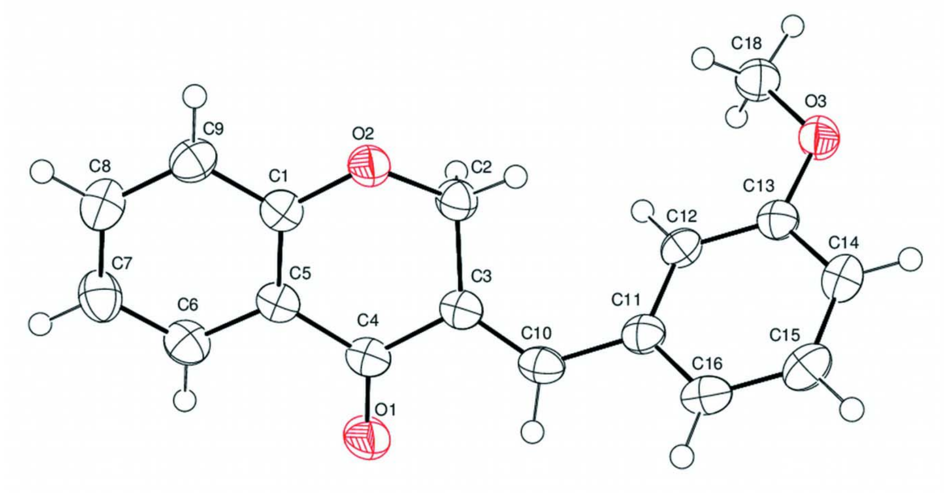

Figure 1

The asymmetric unit of the title compound with displacement ellipsoids drawn at the 50% probability level.

3-(3-Methoxybenzylidene)chroman-4-one

Crystal data

$C_{17}H_{14}O_3$
$M_r = 266.28$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.4143\ (9)$ Å
$b = 6.7141\ (5)$ Å
$c = 16.0031\ (10)$ Å
$\beta = 98.658\ (4)°$
$V = 1318.67\ (16)$ Å^3
$Z = 4$
$F(000) = 560$
$D_x = 1.341$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5379 reflections
$\theta = 2.6–25°$
$\mu = 0.09$ mm^{-1}
$T = 446$ K
Block, colourless
0.28 × 0.21 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Graphite monochromator
φ and ω scans
4414 measured reflections
2315 independent reflections
1662 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\rm max} = 25°$, $\theta_{\rm min} = 2.6°$
$h = -14\rightarrow14$
$k = -7\rightarrow7$
$l = -19\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.112$
$S = 1.00$
2315 reflections
182 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0753P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.21$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.20$ e Å^{-3}

Special details

Experimental. Carbon-bound H-atoms were placed in calculated positions [C—H = 0.96 Å for Me H atoms, 0.97 Å for Methylene H atoms and 0.93 Å for aromatic H atoms; U_{iso}(H) = 1.2U_{eq}(C) (1.5 for Me groups)] and were included in the refinement in the riding model approximation.

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 $F^2 > \sigma(F^2)$ 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. The following ALERTS were generated. Each ALERT has the format test-name_ALERT_alert-type_alert-level. PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) ···.. 1 PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/*L*= 0.595 3 PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ···. 3 PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still 46 Perc. Noted

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.67104 (13)	−0.0244 (2)	0.41235 (9)	0.0308 (4)
C2	0.48754 (13)	0.0872 (2)	0.36955 (9)	0.0345 (4)
H2A	0.4209	0.0984	0.3941	0.041*
H2B	0.47	0.0197	0.3156	0.041*
C3	0.52909 (12)	0.2927 (2)	0.35484 (8)	0.0311 (4)
C4	0.64423 (13)	0.3033 (2)	0.33980 (9)	0.0334 (4)
C5	0.71355 (12)	0.1319 (2)	0.36945 (9)	0.0309 (4)
C6	0.82476 (13)	0.1305 (2)	0.36328 (9)	0.0384 (4)
H6	0.8537	0.2318	0.3338	0.046*
C7	0.89190 (15)	−0.0181 (2)	0.40005 (10)	0.0431 (4)
H7	0.9659	−0.0166	0.3963	0.052*
C8	0.84792 (14)	−0.1708 (2)	0.44296 (10)	0.0425 (4)
H8	0.8933	−0.2712	0.4681	0.051*
C9	0.73865 (13)	−0.1761 (2)	0.44890 (9)	0.0368 (4)
H9	0.7102	−0.2801	0.4771	0.044*
C10	0.47198 (13)	0.4614 (2)	0.35582 (8)	0.0332 (4)
H10	0.5096	0.578	0.3479	0.04*
C11	0.35772 (13)	0.4872 (2)	0.36769 (9)	0.0319 (4)
C12	0.27627 (12)	0.3537 (2)	0.33279 (8)	0.0302 (4)
H12	0.2937	0.2466	0.3005	0.036*
C13	0.16990 (12)	0.3818 (2)	0.34652 (8)	0.0307 (4)
C14	0.14246 (14)	0.5448 (2)	0.39277 (9)	0.0360 (4)
H14	0.0707	0.5638	0.4012	0.043*
C15	0.22209 (14)	0.6782 (2)	0.42606 (9)	0.0387 (4)
H15	0.2038	0.787	0.457	0.046*
C16	0.32907 (14)	0.6509 (2)	0.41361 (9)	0.0364 (4)
H16	0.3822	0.7419	0.4359	0.044*
C18	0.11018 (14)	0.0863 (2)	0.27058 (10)	0.0392 (4)
H18A	0.1373	0.1281	0.2203	0.059*
H18B	0.0455	0.008	0.2554	0.059*
H18C	0.1645	0.0078	0.3048	0.059*

O1	0.68030 (9)	0.45005 (16)	0.30738 (7)	0.0461 (3)
O2	0.56502 (9)	−0.03170 (14)	0.42472 (6)	0.0357 (3)
O3	0.08530 (8)	0.25717 (14)	0.31708 (6)	0.0377 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0339 (10)	0.0333 (8)	0.0255 (7)	−0.0017 (7)	0.0053 (7)	−0.0052 (6)
C2	0.0318 (9)	0.0358 (9)	0.0349 (8)	−0.0019 (7)	0.0023 (7)	0.0042 (7)
C3	0.0340 (10)	0.0331 (8)	0.0250 (7)	−0.0038 (7)	0.0010 (7)	0.0028 (6)
C4	0.0364 (10)	0.0350 (8)	0.0284 (8)	−0.0060 (7)	0.0033 (7)	0.0012 (7)
C5	0.0338 (10)	0.0342 (8)	0.0246 (7)	−0.0045 (7)	0.0043 (6)	−0.0018 (6)
C6	0.0393 (11)	0.0442 (9)	0.0328 (8)	−0.0033 (8)	0.0095 (7)	0.0036 (7)
C7	0.0347 (10)	0.0541 (10)	0.0421 (9)	0.0034 (8)	0.0115 (8)	0.0024 (8)
C8	0.0436 (12)	0.0450 (10)	0.0395 (9)	0.0096 (8)	0.0082 (8)	0.0036 (7)
C9	0.0440 (11)	0.0340 (8)	0.0331 (8)	0.0016 (8)	0.0086 (7)	0.0027 (7)
C10	0.0371 (10)	0.0318 (8)	0.0295 (8)	−0.0079 (7)	0.0014 (7)	0.0039 (6)
C11	0.0369 (10)	0.0295 (8)	0.0285 (7)	−0.0001 (7)	0.0031 (7)	0.0063 (6)
C12	0.0357 (10)	0.0273 (8)	0.0272 (7)	0.0025 (7)	0.0033 (7)	0.0006 (6)
C13	0.0327 (10)	0.0304 (8)	0.0279 (7)	−0.0003 (7)	0.0012 (7)	0.0029 (7)
C14	0.0376 (10)	0.0369 (9)	0.0337 (8)	0.0075 (7)	0.0058 (7)	−0.0005 (7)
C15	0.0505 (12)	0.0320 (8)	0.0328 (8)	0.0067 (8)	0.0036 (8)	−0.0029 (7)
C16	0.0459 (11)	0.0281 (8)	0.0331 (8)	−0.0049 (7)	−0.0006 (7)	0.0016 (7)
C18	0.0399 (10)	0.0356 (9)	0.0414 (9)	−0.0022 (7)	0.0035 (8)	−0.0060 (7)
O1	0.0398 (7)	0.0450 (7)	0.0544 (7)	−0.0050 (5)	0.0104 (6)	0.0163 (6)
O2	0.0322 (7)	0.0353 (6)	0.0399 (6)	−0.0008 (5)	0.0064 (5)	0.0092 (5)
O3	0.0320 (7)	0.0366 (6)	0.0442 (6)	0.0002 (5)	0.0051 (5)	−0.0072 (5)

Geometric parameters (Å, º)

C1—O2	1.3610 (18)	C9—H9	0.93
C1—C9	1.391 (2)	C10—C11	1.469 (2)
C1—C5	1.400 (2)	C10—H10	0.93
C2—O2	1.4443 (18)	C11—C16	1.397 (2)
C2—C3	1.504 (2)	C11—C12	1.403 (2)
C2—H2A	0.97	C12—C13	1.384 (2)
C2—H2B	0.97	C12—H12	0.93
C3—C10	1.337 (2)	C13—O3	1.3697 (18)
C3—C4	1.487 (2)	C13—C14	1.392 (2)
C4—O1	1.2290 (16)	C14—C15	1.380 (2)
C4—C5	1.472 (2)	C14—H14	0.93
C5—C6	1.399 (2)	C15—C16	1.384 (2)
C6—C7	1.375 (2)	C15—H15	0.93
C6—H6	0.93	C16—H16	0.93
C7—C8	1.391 (2)	C18—O3	1.4264 (16)
C7—H7	0.93	C18—H18A	0.96
C8—C9	1.374 (2)	C18—H18B	0.96
C8—H8	0.93	C18—H18C	0.96
O2—C1—C9	116.60 (12)	C3—C10—C11	128.70 (13)

O2—C1—C5	122.87 (13)	C3—C10—H10	115.6
C9—C1—C5	120.44 (14)	C11—C10—H10	115.6
O2—C2—C3	112.97 (13)	C16—C11—C12	119.11 (14)
O2—C2—H2A	109	C16—C11—C10	119.20 (14)
C3—C2—H2A	109	C12—C11—C10	121.68 (13)
O2—C2—H2B	109	C13—C12—C11	119.85 (13)
C3—C2—H2B	109	C13—C12—H12	120.1
H2A—C2—H2B	107.8	C11—C12—H12	120.1
C10—C3—C4	119.08 (13)	O3—C13—C12	124.26 (13)
C10—C3—C2	125.45 (14)	O3—C13—C14	115.26 (13)
C4—C3—C2	115.46 (13)	C12—C13—C14	120.48 (14)
O1—C4—C5	122.03 (14)	C15—C14—C13	119.80 (15)
O1—C4—C3	121.80 (13)	C15—C14—H14	120.1
C5—C4—C3	116.12 (12)	C13—C14—H14	120.1
C6—C5—C1	118.60 (14)	C14—C15—C16	120.36 (14)
C6—C5—C4	121.17 (13)	C14—C15—H15	119.8
C1—C5—C4	119.92 (13)	C16—C15—H15	119.8
C7—C6—C5	121.05 (14)	C15—C16—C11	120.37 (15)
C7—C6—H6	119.5	C15—C16—H16	119.8
C5—C6—H6	119.5	C11—C16—H16	119.8
C6—C7—C8	119.27 (15)	O3—C18—H18A	109.5
C6—C7—H7	120.4	O3—C18—H18B	109.5
C8—C7—H7	120.4	H18A—C18—H18B	109.5
C9—C8—C7	121.20 (15)	O3—C18—H18C	109.5
C9—C8—H8	119.4	H18A—C18—H18C	109.5
C7—C8—H8	119.4	H18B—C18—H18C	109.5
C8—C9—C1	119.43 (14)	C1—O2—C2	117.43 (10)
C8—C9—H9	120.3	C13—O3—C18	117.11 (11)
C1—C9—H9	120.3		

O2—C2—C3—C10	−136.04 (14)	C5—C1—C9—C8	0.3 (2)
O2—C2—C3—C4	42.74 (17)	C4—C3—C10—C11	178.71 (13)
C10—C3—C4—O1	−19.0 (2)	C2—C3—C10—C11	−2.6 (2)
C2—C3—C4—O1	162.15 (13)	C3—C10—C11—C16	143.03 (15)
C10—C3—C4—C5	158.36 (13)	C3—C10—C11—C12	−38.1 (2)
C2—C3—C4—C5	−20.50 (18)	C16—C11—C12—C13	−2.14 (19)
O2—C1—C5—C6	177.14 (12)	C10—C11—C12—C13	179.04 (12)
C9—C1—C5—C6	0.8 (2)	C11—C12—C13—O3	−178.24 (12)
O2—C1—C5—C4	3.5 (2)	C11—C12—C13—C14	1.8 (2)
C9—C1—C5—C4	−172.79 (13)	O3—C13—C14—C15	179.26 (12)
O1—C4—C5—C6	1.2 (2)	C12—C13—C14—C15	−0.8 (2)
C3—C4—C5—C6	−176.16 (12)	C13—C14—C15—C16	0.1 (2)
O1—C4—C5—C1	174.63 (13)	C14—C15—C16—C11	−0.4 (2)
C3—C4—C5—C1	−2.72 (19)	C12—C11—C16—C15	1.5 (2)
C1—C5—C6—C7	−1.5 (2)	C10—C11—C16—C15	−179.69 (13)
C4—C5—C6—C7	172.06 (14)	C9—C1—O2—C2	−163.08 (12)
C5—C6—C7—C8	0.9 (2)	C5—C1—O2—C2	20.46 (18)
C6—C7—C8—C9	0.3 (2)	C3—C2—O2—C1	−43.00 (16)
C7—C8—C9—C1	−0.9 (2)	C12—C13—O3—C18	1.11 (19)

O2—C1—C9—C8	−176.20 (13)	C14—C13—O3—C18	−178.95 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*B*···O1^{i}	0.97	2.54	3.3808 (19)	145
C18—H18*B*···O3^{ii}	0.96	2.50	3.4227 (19)	161

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*, *y*−1/2, −*z*+1/2.