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7-(6-Bromohexyloxy)-4-methyl-2*H*-chromen-2-one

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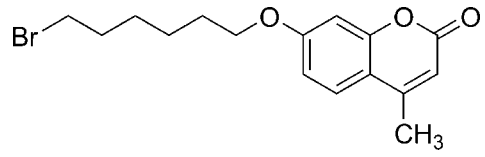
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.115; data-to-parameter ratio = 16.9.

In the title molecule, $C_{16}H_{19}BrO_3$, all non-H atoms apart from the Br atom are approximately coplanar, with a maximum deviation of 0.242 (4) Å. The C—C—C—Br torsion angle is 66.5 (4)°.

Related literature

For the pharmacological activity of coumarin compounds, see: Wu *et al.* (2009); Shi & Zhou (2011). For details of the synthesis, see: Shi *et al.* (2011). For a related structure, see: Zhang *et al.* (2011).



Experimental

Crystal data

$C_{16}H_{19}BrO_3$
M_r = 339.22
Monoclinic, $C2/c$
a = 15.681 (5) Å
b = 9.540 (3) Å
c = 22.104 (7) Å
β = 110.201 (6)°
V = 3103.3 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.65 mm^{-1}
T = 296 K
0.22 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.593, T_{max} = 0.692
8381 measured reflections
3051 independent reflections
1921 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.115
S = 1.01
3051 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Data collection: *APEX2* (Sheldrick, 2008); cell refinement: *SAINT* (Sheldrick, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5459).

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Wu, L., Wang, X., Xu, W., Farzaneh, F. & Xu, R. (2009). *Curr. Med. Chem.* **16**, 4236–4260.
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supporting information

Acta Cryst. (2012). E**68**, o1709 [doi:10.1107/S1600536812020442]

7-(6-Bromohexyloxy)-4-methyl-2*H*-chromen-2-one

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S1. Comment

Coumarin compounds are important in medicinal chemistry due to their extensive potential applications in antibacterial, antifungal, antiviral, anti-tubercular, anti-malarial, anticancer and anti-inflammatory fields (Wu, *et al.*, 2009; Shi & Zhou, 2011). Our interest is to develop novel coumarin compounds as antimicrobial agents and some structral related coumarin-triazoles have been reported as potential bioactive agents (Shi, *et al.*, 2011; Zhang, *et al.*, 2011). Herein, we report the crystal structure of the title compound (I).

The molecular structure of (I) is shown in Fig. 1. With the exception of the Br atom, all non-hydrogen atoms are approximately co-planar with a maximum deviation of 0.242 (4)Å (C16). The C14—C15—C16—Br1 torsion angle is 66.5 (4)Å.

S2. Experimental

Compound (I) was prepared according to the procedure of Shi & Zhou (2011). Single crystals were grown by slow evaporation of a solution of (I) in $CHCl_3$ at room temperature.

S3. Refinement

H atoms were placed at calculated position with C—H = 0.93 Å (aromatic), 0.96 Å (methyl) and 0.97 Å (methylene). The U_{iso}(H) values were set to 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

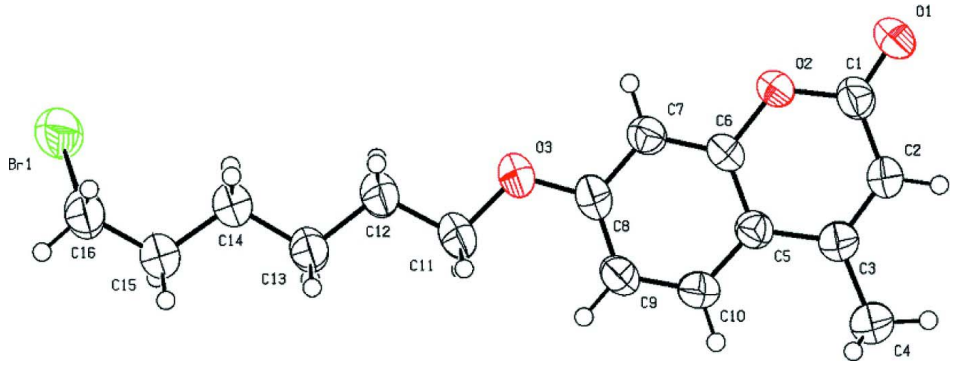

Figure 1

The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level.

7-(6-Bromohexyloxy)-4-methyl-2*H*-chromen-2-one

Crystal data

$C_{16}H_{19}BrO_3$
M_r = 339.22

Monoclinic, *C*2/*c*
Hall symbol: -C 2yc

a = 15.681 (5) Å
b = 9.540 (3) Å
c = 22.104 (7) Å
β = 110.201 (6)°
V = 3103.3 (18) Å^3
Z = 8
F(000) = 1392
D_x = 1.452 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2005 reflections
θ = 2.6–22.1°
μ = 2.65 mm^{-1}
T = 296 K
Block, colorless
0.22 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.593, T_{max} = 0.692

8381 measured reflections
3051 independent reflections
1921 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 26.0°, θ_{min} = 2.5°
h = −19→19
k = −9→11
l = −27→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.115
S = 1.01
3051 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 2.7774P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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.

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

	x	y	z	U_{iso}*/U_{eq}
Br1	0.13272 (3)	0.92653 (5)	0.02243 (2)	0.0880 (2)
C1	0.7117 (2)	−0.1670 (3)	0.24911 (16)	0.0537 (8)
C2	0.6618 (2)	−0.2939 (3)	0.22745 (15)	0.0545 (8)
H2A	0.6926	−0.3787	0.2379	0.065*
C3	0.5727 (2)	−0.2965 (3)	0.19283 (15)	0.0513 (8)
C4	0.5235 (3)	−0.4315 (3)	0.1708 (2)	0.0741 (11)
H4A	0.5654	−0.5082	0.1847	0.111*
H4B	0.4973	−0.4319	0.1246	0.111*
H4C	0.4763	−0.4412	0.1889	0.111*

C5	0.5242 (2)	−0.1647 (3)	0.17747 (14)	0.0442 (7)
C6	0.57263 (19)	−0.0413 (3)	0.19839 (14)	0.0427 (7)
C7	0.5329 (2)	0.0882 (3)	0.18675 (15)	0.0478 (7)
H7A	0.5674	0.1687	0.2012	0.057*
C8	0.4408 (2)	0.0971 (3)	0.15309 (15)	0.0514 (8)
C9	0.3895 (2)	−0.0240 (3)	0.13091 (15)	0.0527 (8)
H9A	0.3274	−0.0181	0.1083	0.063*
C10	0.4319 (2)	−0.1512 (3)	0.14297 (15)	0.0528 (8)
H10A	0.3978	−0.2316	0.1275	0.063*
C11	0.3099 (2)	0.2471 (3)	0.11206 (17)	0.0602 (9)
H11A	0.2765	0.1966	0.1348	0.072*
H11B	0.2915	0.2118	0.0683	0.072*
C12	0.2914 (2)	0.4009 (3)	0.11200 (19)	0.0612 (9)
H12A	0.3306	0.4497	0.0932	0.073*
H12B	0.3073	0.4324	0.1563	0.073*
C13	0.1935 (2)	0.4414 (3)	0.07516 (16)	0.0557 (8)
H13A	0.1779	0.4142	0.0303	0.067*
H13B	0.1537	0.3911	0.0928	0.067*
C14	0.1785 (2)	0.5971 (3)	0.07899 (17)	0.0584 (9)
H14A	0.1936	0.6231	0.1239	0.070*
H14B	0.2199	0.6466	0.0625	0.070*
C15	0.0828 (2)	0.6447 (3)	0.04209 (17)	0.0579 (8)
H15A	0.0713	0.6332	−0.0036	0.069*
H15B	0.0407	0.5844	0.0533	0.069*
C16	0.0638 (2)	0.7941 (4)	0.05454 (19)	0.0674 (10)
H16A	0.0790	0.8079	0.1005	0.081*
H16B	−0.0006	0.8128	0.0339	0.081*
O1	0.79161 (16)	−0.1577 (2)	0.27985 (13)	0.0766 (8)
O2	0.66442 (13)	−0.0436 (2)	0.23286 (10)	0.0503 (5)
O3	0.40587 (14)	0.2292 (2)	0.14399 (12)	0.0649 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0703 (3)	0.0743 (3)	0.1032 (4)	0.0001 (2)	0.0092 (2)	0.0270 (2)
C1	0.0448 (19)	0.053 (2)	0.059 (2)	0.0053 (15)	0.0121 (16)	0.0118 (16)
C2	0.047 (2)	0.0450 (18)	0.063 (2)	0.0062 (15)	0.0084 (16)	0.0043 (15)
C3	0.050 (2)	0.0476 (18)	0.0523 (19)	0.0003 (14)	0.0122 (15)	−0.0034 (15)
C4	0.061 (2)	0.055 (2)	0.088 (3)	0.0001 (17)	0.003 (2)	−0.0139 (19)
C5	0.0413 (17)	0.0469 (17)	0.0416 (16)	0.0011 (13)	0.0107 (14)	−0.0022 (13)
C6	0.0331 (16)	0.0509 (18)	0.0416 (17)	0.0017 (13)	0.0097 (13)	0.0029 (13)
C7	0.0411 (17)	0.0485 (18)	0.0521 (19)	−0.0018 (14)	0.0141 (14)	0.0044 (14)
C8	0.0445 (18)	0.056 (2)	0.0533 (19)	0.0111 (15)	0.0160 (15)	0.0096 (15)
C9	0.0376 (17)	0.059 (2)	0.0545 (19)	0.0040 (15)	0.0065 (15)	−0.0024 (16)
C10	0.0442 (18)	0.0516 (19)	0.057 (2)	−0.0047 (14)	0.0096 (15)	−0.0085 (15)
C11	0.0435 (19)	0.064 (2)	0.070 (2)	0.0135 (16)	0.0152 (16)	0.0051 (18)
C12	0.048 (2)	0.057 (2)	0.077 (2)	0.0098 (15)	0.0192 (18)	0.0057 (17)
C13	0.0495 (19)	0.057 (2)	0.058 (2)	0.0099 (15)	0.0151 (16)	0.0016 (16)

C14	0.0501 (19)	0.055 (2)	0.065 (2)	0.0062 (15)	0.0135 (17)	0.0026 (16)
C15	0.052 (2)	0.056 (2)	0.063 (2)	0.0062 (16)	0.0154 (17)	0.0027 (16)
C16	0.057 (2)	0.065 (2)	0.080 (3)	0.0135 (17)	0.0220 (19)	0.0094 (19)
O1	0.0404 (14)	0.0630 (16)	0.104 (2)	0.0007 (11)	−0.0028 (14)	0.0119 (14)
O2	0.0358 (12)	0.0467 (12)	0.0610 (14)	−0.0013 (9)	0.0070 (10)	0.0049 (10)
O3	0.0437 (13)	0.0537 (13)	0.0888 (17)	0.0102 (10)	0.0120 (12)	0.0073 (12)

Geometric parameters (Å, º)

Br1—C16	1.949 (4)	C9—H9A	0.9300
C1—O1	1.205 (4)	C10—H10A	0.9300
C1—O2	1.371 (4)	C11—O3	1.435 (4)
C1—C2	1.431 (4)	C11—C12	1.496 (4)
C2—C3	1.341 (4)	C11—H11A	0.9700
C2—H2A	0.9300	C11—H11B	0.9700
C3—C5	1.448 (4)	C12—C13	1.520 (4)
C3—C4	1.494 (4)	C12—H12A	0.9700
C4—H4A	0.9600	C12—H12B	0.9700
C4—H4B	0.9600	C13—C14	1.511 (4)
C4—H4C	0.9600	C13—H13A	0.9700
C5—C6	1.391 (4)	C13—H13B	0.9700
C5—C10	1.390 (4)	C14—C15	1.510 (4)
C6—O2	1.377 (3)	C14—H14A	0.9700
C6—C7	1.367 (4)	C14—H14B	0.9700
C7—C8	1.380 (4)	C15—C16	1.501 (5)
C7—H7A	0.9300	C15—H15A	0.9700
C8—O3	1.362 (4)	C15—H15B	0.9700
C8—C9	1.397 (4)	C16—H16A	0.9700
C9—C10	1.365 (4)	C16—H16B	0.9700
O1—C1—O2	116.6 (3)	O3—C11—H11B	110.4
O1—C1—C2	126.4 (3)	C12—C11—H11B	110.4
O2—C1—C2	117.0 (3)	H11A—C11—H11B	108.6
C3—C2—C1	123.2 (3)	C11—C12—C13	114.1 (3)
C3—C2—H2A	118.4	C11—C12—H12A	108.7
C1—C2—H2A	118.4	C13—C12—H12A	108.7
C2—C3—C5	118.5 (3)	C11—C12—H12B	108.7
C2—C3—C4	121.4 (3)	C13—C12—H12B	108.7
C5—C3—C4	120.1 (3)	H12A—C12—H12B	107.6
C3—C4—H4A	109.5	C14—C13—C12	111.6 (3)
C3—C4—H4B	109.5	C14—C13—H13A	109.3
H4A—C4—H4B	109.5	C12—C13—H13A	109.3
C3—C4—H4C	109.5	C14—C13—H13B	109.3
H4A—C4—H4C	109.5	C12—C13—H13B	109.3
H4B—C4—H4C	109.5	H13A—C13—H13B	108.0
C6—C5—C10	116.7 (3)	C15—C14—C13	114.2 (3)
C6—C5—C3	118.4 (3)	C15—C14—H14A	108.7
C10—C5—C3	124.9 (3)	C13—C14—H14A	108.7

O2—C6—C7	116.1 (3)	C15—C14—H14B	108.7
O2—C6—C5	121.1 (3)	C13—C14—H14B	108.7
C7—C6—C5	122.8 (3)	H14A—C14—H14B	107.6
C8—C7—C6	118.7 (3)	C16—C15—C14	114.2 (3)
C8—C7—H7A	120.6	C16—C15—H15A	108.7
C6—C7—H7A	120.6	C14—C15—H15A	108.7
O3—C8—C7	115.5 (3)	C16—C15—H15B	108.7
O3—C8—C9	124.1 (3)	C14—C15—H15B	108.7
C7—C8—C9	120.5 (3)	H15A—C15—H15B	107.6
C10—C9—C8	118.9 (3)	C15—C16—Br1	112.3 (2)
C10—C9—H9A	120.5	C15—C16—H16A	109.2
C8—C9—H9A	120.5	Br1—C16—H16A	109.2
C9—C10—C5	122.3 (3)	C15—C16—H16B	109.2
C9—C10—H10A	118.8	Br1—C16—H16B	109.2
C5—C10—H10A	118.8	H16A—C16—H16B	107.9
O3—C11—C12	106.6 (3)	C1—O2—C6	121.8 (2)
O3—C11—H11A	110.4	C8—O3—C11	118.9 (3)
C12—C11—H11A	110.4		

O1—C1—C2—C3	−179.4 (3)	C7—C8—C9—C10	−0.1 (5)
O2—C1—C2—C3	−0.1 (5)	C8—C9—C10—C5	1.1 (5)
C1—C2—C3—C5	−1.1 (5)	C6—C5—C10—C9	−1.3 (5)
C1—C2—C3—C4	179.5 (3)	C3—C5—C10—C9	178.8 (3)
C2—C3—C5—C6	1.1 (4)	O3—C11—C12—C13	175.4 (3)
C4—C3—C5—C6	−179.5 (3)	C11—C12—C13—C14	177.9 (3)
C2—C3—C5—C10	−179.0 (3)	C12—C13—C14—C15	178.8 (3)
C4—C3—C5—C10	0.5 (5)	C13—C14—C15—C16	170.5 (3)
C10—C5—C6—O2	−179.9 (3)	C14—C15—C16—Br1	66.5 (4)
C3—C5—C6—O2	0.0 (4)	O1—C1—O2—C6	−179.3 (3)
C10—C5—C6—C7	0.5 (4)	C2—C1—O2—C6	1.3 (4)
C3—C5—C6—C7	−179.5 (3)	C7—C6—O2—C1	178.3 (3)
O2—C6—C7—C8	−179.2 (3)	C5—C6—O2—C1	−1.3 (4)
C5—C6—C7—C8	0.3 (5)	C7—C8—O3—C11	−177.1 (3)
C6—C7—C8—O3	179.3 (3)	C9—C8—O3—C11	2.7 (5)
C6—C7—C8—C9	−0.6 (5)	C12—C11—O3—C8	177.3 (3)
O3—C8—C9—C10	−179.9 (3)		