IUCrData

ISSN 2414-3146

2-Oxo-2*H*-chromen-7-yl 3-methylbutanoate

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Received 13 January 2025
Accepted 21 February 2025

Edited by S. Bernès, Benemérita Universidad Autónoma de Puebla, México

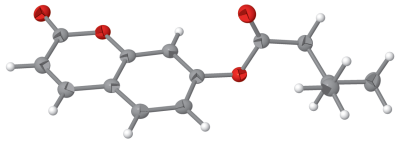
Keywords: crystal structure; coumarin derivative; umbelliferone; hydrogen bonds.

CCDC reference: 2426608

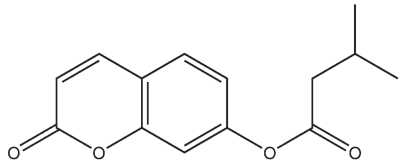
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{14}H_{14}O_4$, was synthesized by *O*-acylation of umbelliferone with isovaleryl chloride in the presence of diethyl ether as a solvent and pyridine as a base. The side chain moiety *i.e.* the acetate fragment linking to the methylethyl group is almost orthogonal to the almost planar (r.m.s deviation = 0.020 Å) coumarin ring system, making an angle of 76.26 (7)°. In the crystal, the molecules form centrosymmetric dimers through pairwise C—H···O hydrogen bonds, generating $R_2^2(8)$ and $R_2^2(18)$ loops that lie within the crystallographic *ac* plane and propagate along the [001] direction.

3D view



Chemical scheme



Structure description

Molecules containing the coumarin moiety have attracted the attention of researchers since examples of these compounds have been shown to have extensive biological properties, including anti-HIV (Yu *et al.*, 2003, 2007), anti-coagulant (Abernethy *et al.*, 1969), anti-oxidant (Vukovic *et al.*, 2010), anti-tumour (Basanagouda *et al.*, 2009), anti-bacterial (Vukovic *et al.*, 2010) and anti-inflammatory (Emmanuel-Giota *et al.*, 2001) activity. They are also used in the perfumery and agrochemical industries as activators and stabilizers (Bauer *et al.*, 1988; Boisde & Meuly, 1993).

IIn this work, we describe the synthesis and structure of the title compound, $C_{14}H_{14}O_4$, Fig. 1. An analysis of the bond lengths in this structure shows a slightly uneven distribution around the pyrone ring, as indicated by the lengths of the C2═C3 [1.345 (3) Å] and C1—C2 [1.453 (3) Å] bonds, which are shorter and longer, respectively, than what would be expected for a $C_{ar}—C_{ar}$ bond. This suggests that the electron density is less concentrated in the C2═C3 bond of the pyran-2-one ring, resulting in the formation of a

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O4^{i}	0.98 (3)	2.46 (3)	3.296 (2)	142.6 (19)
C6—H5···O1^{ii}	0.96 (3)	2.51 (3)	3.444 (2)	167 (2)
C11—H11A···O2^{ii}	1.03 (3)	2.60 (3)	3.245 (2)	120.5 (18)

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, -y, -z+1$.

double bond, as observed in other coumarin ester derivatives (Abou *et al.*, 2020; Koulabiga *et al.*, 2024; Yao *et al.*, 2024). Furthermore, the structure highlights an almost planar coumarin ring system (puckering τ parameter = 0.7; Spek, 2009). Likewise, the crystal structure reveals the generation of dimeric units *via* C—H···O interactions. These dimers are linked by further C—H···O contacts into chains along the [001] direction (Table 1, Fig. 2).

Synthesis and crystallization

To a solution of isovaleryl chloride (0.76 ml, 6.17 mmol, 1 equiv.) in dried diethyl ether (16 ml) was added dried pyridine (2.31 ml, 4.7 equiv.) and umbelliferone (1 g, 6.17 mmol, 1 equiv.) in small portions over 30 min, with vigorous stirring. The reaction mixture was left stirring at room temperature for 3 h. The resulting mixture was next poured into a separating funnel containing 40 ml of chloroform and washed with diluted hydrochloric acid solution until the pH was 2–3. The organic phase was extracted, washed with water to neutrality, dried with magnesium sulfate and the solvent removed *in vacuo*. The obtained crude product was filtered off with suction, washed with petroleum ether and recrystallized from the mixed solvents of chloroform–hexane (1:3), yielding a white powder of the title compound, 2-oxo-2*H*-chromen-7-yl-3-methylbutanoate (0.92 g, 60%). Colourless crystals suitable for single-crystal X-ray diffraction analysis were then obtained from an acetone solution, after the solvent was allowed to evaporate slowly at ambient conditions.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Three reflections, ($\bar{3}$46), ($\bar{2}$04), ($\bar{1}$04) with $\Delta F/\sigma(F)$ higher than 10, were found to have too low intensities, caused by a systematic error, probably by shielding by the beam-stop interference for reflections ($\bar{2}$04), ($\bar{1}$04) while for ($\bar{3}$46) at higher 2θ angles, the less area irradiated would have an effect of decreasing diffraction intensity. The depth of penetration of the beam becomes commensurably deeper with higher angles. This effectively increases background as well as a sample displacement effect.. They were omitted from the refinement.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{14}O_4$
M_r	246.25
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	15.370 (3), 5.4488 (10), 16.339 (3)
β (°)	117.426 (7)
V (Å^3)	1214.5 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.45 × 0.44 × 0.16
Data collection	
Diffractometer	SuperNova, Dual, Cu at home/near, AtlasS2
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.956, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41227, 3741, 2799
R_{int}	0.068
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.718
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.066, 0.203, 1.03
No. of reflections	41227
No. of parameters	219
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.50, −0.39

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015*a*), *PLATON* (Spek, 2020), *SHELXL2018/3* (Sheldrick, 2015*b*), *publCIF* (Westrip, 2010) and *WinGX* (Farrugia, 2012).

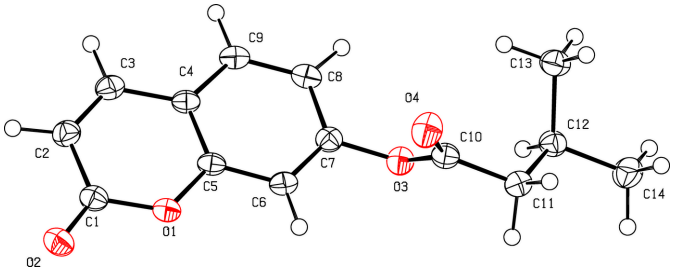


Figure 1
Molecular structure of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

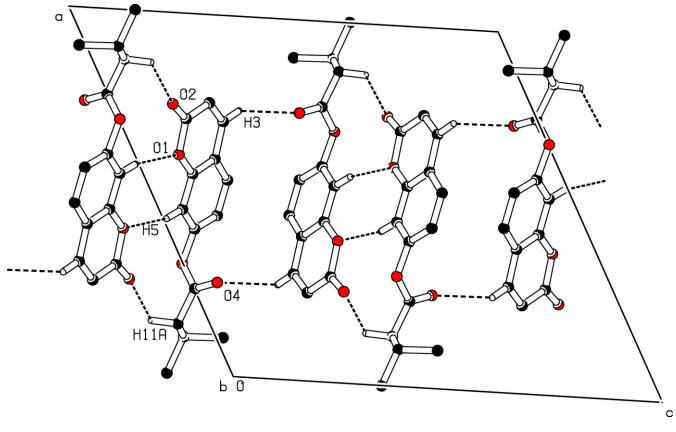


Figure 2
A view of the crystal packing showing the association of molecules into centrosymmetric dimers through C—H···O hydrogen bonds, forming $R_2^2(8)$ and $R_2^2(18)$ loops extending parallel to the *ac* crystallographic plane. H atoms not involved in hydrogen bonding have been omitted for clarity.

Acknowledgements

The authors thank the Institute Jean Barriol (Université de Lorraine, France) for the X-ray diffraction measurements and the AFRAMED project for the crystal structure determination..

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full crystallographic data

IUCrData (2025). **10**, x250161 [https://doi.org/10.1107/S2414314625001610]

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Crystal data

$C_{14}H_{14}O_4$
M_r = 246.25
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 15.370 (3) Å
b = 5.4488 (10) Å
c = 16.339 (3) Å
β = 117.426 (7)°
V = 1214.5 (4) Å^3
Z = 4
$F(000)$ = 520
D_x = 1.347 Mg m^{-3}
Melting point = 341–343 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3741 reflections
θ = 5.0–61.4°
μ = 0.10 mm^{-1}
T = 296 K
Prism, white
0.45 × 0.44 × 0.16 mm

Data collection

SuperNova, Dual, Cu at home/near, AtlasS2 diffractometer
Radiation source: micro-focus sealed X-ray tube
Mirror monochromator
Detector resolution: 5.3048 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
T_{min} = 0.956, T_{max} = 1.000
41227 measured reflections
3741 independent reflections
2799 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 30.7°, θ_{min} = 2.5°
h = −22→21
k = −7→7
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.203
S = 1.03
41227 reflections
219 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.1174P)^2 + 0.7176P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Special details

Refinement. All non-H atoms were refined anisotropically. H atoms were located in difference Fourier maps and refined freely with an isotropic displacement parameter.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.30502 (9)	0.5548 (2)	0.49786 (9)	0.0262 (3)
O1	0.60720 (9)	0.1291 (2)	0.60615 (8)	0.0247 (3)
O2	0.74608 (10)	−0.0712 (3)	0.64517 (10)	0.0315 (3)
O4	0.25820 (10)	0.2488 (3)	0.56157 (10)	0.0362 (4)
C5	0.55518 (12)	0.3187 (3)	0.61799 (11)	0.0225 (3)
C4	0.60061 (12)	0.4940 (3)	0.68735 (11)	0.0230 (3)
C7	0.40292 (12)	0.5249 (3)	0.56429 (11)	0.0236 (3)
C6	0.45580 (13)	0.3301 (3)	0.55611 (11)	0.0240 (3)
C3	0.70488 (13)	0.4686 (3)	0.74636 (12)	0.0268 (4)
C11	0.13750 (13)	0.4489 (4)	0.42324 (12)	0.0276 (4)
C1	0.70685 (13)	0.1025 (3)	0.66096 (12)	0.0249 (3)
C12	0.10241 (13)	0.7130 (3)	0.42369 (12)	0.0262 (4)
C10	0.23739 (13)	0.3983 (3)	0.50137 (12)	0.0257 (3)
C9	0.54337 (13)	0.6854 (3)	0.69455 (12)	0.0260 (3)
C2	0.75496 (13)	0.2830 (4)	0.73351 (12)	0.0279 (4)
C8	0.44435 (13)	0.7026 (3)	0.63285 (12)	0.0258 (3)
C14	−0.00084 (16)	0.7484 (4)	0.34503 (14)	0.0361 (4)
C13	0.10591 (15)	0.7726 (4)	0.51641 (14)	0.0312 (4)
H5	0.4273 (19)	0.210 (5)	0.5086 (19)	0.040 (7)*
H3	0.7378 (17)	0.589 (5)	0.7957 (17)	0.036 (6)*
H9	0.5763 (18)	0.811 (5)	0.7445 (19)	0.041 (7)*
H8	0.4032 (18)	0.849 (5)	0.6331 (18)	0.037 (6)*
H2	0.8282 (17)	0.258 (4)	0.7702 (16)	0.027 (6)*
H11A	0.1421 (18)	0.418 (5)	0.3633 (18)	0.039 (7)*
H14A	−0.051 (2)	0.631 (6)	0.352 (2)	0.048 (7)*
H14B	−0.0221 (17)	0.929 (5)	0.3426 (17)	0.034 (6)*
H11B	0.0901 (18)	0.329 (5)	0.4256 (17)	0.035 (6)*
H12	0.1473 (16)	0.826 (4)	0.4176 (15)	0.026 (5)*
H13A	0.0868 (17)	0.946 (5)	0.5179 (17)	0.036 (6)*
H13B	0.1761 (18)	0.750 (4)	0.5683 (18)	0.033 (6)*
H13C	0.059 (2)	0.656 (6)	0.5256 (19)	0.052 (8)*
H14C	−0.005 (2)	0.709 (5)	0.282 (2)	0.051 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0272 (6)	0.0259 (6)	0.0257 (6)	0.0001 (5)	0.0122 (5)	0.0045 (5)
O1	0.0292 (6)	0.0230 (6)	0.0239 (6)	0.0005 (5)	0.0141 (5)	−0.0023 (5)
O2	0.0351 (7)	0.0299 (7)	0.0336 (7)	0.0045 (5)	0.0193 (6)	−0.0002 (5)
O4	0.0338 (7)	0.0409 (8)	0.0323 (7)	−0.0023 (6)	0.0138 (6)	0.0128 (6)
C5	0.0300 (8)	0.0205 (7)	0.0202 (7)	0.0000 (6)	0.0144 (6)	0.0010 (6)
C4	0.0293 (8)	0.0228 (7)	0.0196 (7)	−0.0012 (6)	0.0136 (6)	0.0009 (6)
C7	0.0266 (8)	0.0250 (8)	0.0211 (7)	−0.0005 (6)	0.0126 (6)	0.0031 (6)
C6	0.0291 (8)	0.0233 (8)	0.0205 (7)	−0.0021 (6)	0.0123 (6)	−0.0010 (6)
C3	0.0309 (8)	0.0291 (8)	0.0207 (7)	−0.0023 (7)	0.0121 (6)	−0.0005 (6)

C11	0.0277 (8)	0.0298 (9)	0.0241 (8)	0.0000 (7)	0.0108 (6)	−0.0022 (7)
C1	0.0301 (8)	0.0245 (8)	0.0234 (7)	0.0009 (6)	0.0152 (6)	0.0034 (6)
C12	0.0278 (8)	0.0281 (8)	0.0246 (8)	0.0000 (6)	0.0138 (6)	0.0015 (6)
C10	0.0289 (8)	0.0259 (8)	0.0242 (8)	−0.0002 (6)	0.0139 (6)	0.0008 (6)
C9	0.0336 (8)	0.0239 (8)	0.0228 (7)	−0.0022 (6)	0.0150 (7)	−0.0033 (6)
C2	0.0287 (8)	0.0318 (9)	0.0224 (8)	−0.0005 (7)	0.0112 (6)	0.0009 (7)
C8	0.0341 (9)	0.0226 (8)	0.0254 (8)	0.0011 (6)	0.0177 (7)	0.0000 (6)
C14	0.0345 (10)	0.0391 (11)	0.0289 (9)	0.0071 (8)	0.0097 (8)	0.0023 (8)
C13	0.0348 (9)	0.0335 (10)	0.0294 (9)	−0.0013 (7)	0.0184 (8)	−0.0033 (7)

Geometric parameters (Å, º)

O3—C10	1.366 (2)	C11—H11A	1.03 (3)
O3—C7	1.402 (2)	C11—H11B	0.99 (3)
O1—C5	1.373 (2)	C1—C2	1.453 (3)
O1—C1	1.380 (2)	C12—C14	1.526 (3)
O2—C1	1.212 (2)	C12—C13	1.526 (3)
O4—C10	1.201 (2)	C12—H12	0.96 (2)
C5—C6	1.392 (2)	C9—C8	1.388 (3)
C5—C4	1.398 (2)	C9—H9	1.00 (3)
C4—C9	1.404 (2)	C2—H2	1.01 (2)
C4—C3	1.447 (2)	C8—H8	1.02 (3)
C7—C6	1.380 (2)	C14—H14A	1.04 (3)
C7—C8	1.393 (2)	C14—H14B	1.03 (3)
C6—H5	0.96 (3)	C14—H14C	1.03 (3)
C3—C2	1.345 (3)	C13—H13A	0.99 (3)
C3—H3	0.98 (3)	C13—H13B	1.03 (2)
C11—C10	1.502 (2)	C13—H13C	1.03 (3)
C11—C12	1.538 (3)		
C10—O3—C7	117.47 (13)	C13—C12—C11	110.59 (15)
C5—O1—C1	122.11 (13)	C14—C12—H12	110.5 (13)
O1—C5—C6	116.52 (14)	C13—C12—H12	105.5 (13)
O1—C5—C4	121.48 (15)	C11—C12—H12	109.0 (14)
C6—C5—C4	121.98 (15)	O4—C10—O3	122.46 (16)
C5—C4—C9	118.50 (16)	O4—C10—C11	127.06 (17)
C5—C4—C3	117.45 (15)	O3—C10—C11	110.44 (15)
C9—C4—C3	124.04 (16)	C8—C9—C4	120.59 (16)
C6—C7—C8	122.74 (16)	C8—C9—H9	121.2 (15)
C6—C7—O3	118.98 (15)	C4—C9—H9	118.2 (15)
C8—C7—O3	118.16 (15)	C3—C2—C1	121.56 (17)
C7—C6—C5	117.53 (15)	C3—C2—H2	124.7 (13)
C7—C6—H5	122.5 (15)	C1—C2—H2	113.7 (13)
C5—C6—H5	119.9 (15)	C9—C8—C7	118.63 (16)
C2—C3—C4	120.40 (16)	C9—C8—H8	121.7 (15)
C2—C3—H3	121.0 (14)	C7—C8—H8	119.5 (15)
C4—C3—H3	118.6 (14)	C12—C14—H14A	111.2 (16)
C10—C11—C12	113.02 (15)	C12—C14—H14B	109.9 (13)

C10—C11—H11A	106.7 (14)	H14A—C14—H14B	111 (2)
C12—C11—H11A	109.6 (15)	C12—C14—H14C	112.4 (16)
C10—C11—H11B	109.1 (14)	H14A—C14—H14C	106 (2)
C12—C11—H11B	110.5 (15)	H14B—C14—H14C	107 (2)
H11A—C11—H11B	108 (2)	C12—C13—H13A	110.6 (15)
O2—C1—O1	117.13 (16)	C12—C13—H13B	109.7 (14)
O2—C1—C2	125.87 (17)	H13A—C13—H13B	107.9 (19)
O1—C1—C2	116.99 (15)	C12—C13—H13C	108.1 (16)
C14—C12—C13	110.90 (16)	H13A—C13—H13C	110 (2)
C14—C12—C11	110.18 (15)	H13B—C13—H13C	110 (2)
C1—O1—C5—C6	177.72 (14)	C5—O1—C1—C2	0.9 (2)
C1—O1—C5—C4	−0.8 (2)	C10—C11—C12—C14	−177.74 (16)
O1—C5—C4—C9	178.90 (14)	C10—C11—C12—C13	−54.8 (2)
C6—C5—C4—C9	0.5 (2)	C7—O3—C10—O4	4.3 (3)
O1—C5—C4—C3	0.1 (2)	C7—O3—C10—C11	−177.61 (14)
C6—C5—C4—C3	−178.32 (15)	C12—C11—C10—O4	119.0 (2)
C10—O3—C7—C6	74.6 (2)	C12—C11—C10—O3	−58.91 (19)
C10—O3—C7—C8	−109.20 (18)	C5—C4—C9—C8	−1.4 (3)
C8—C7—C6—C5	−2.0 (3)	C3—C4—C9—C8	177.38 (16)
O3—C7—C6—C5	174.03 (14)	C4—C3—C2—C1	−0.2 (3)
O1—C5—C6—C7	−177.36 (14)	O2—C1—C2—C3	−179.25 (18)
C4—C5—C6—C7	1.1 (2)	O1—C1—C2—C3	−0.4 (3)
C5—C4—C3—C2	0.4 (2)	C4—C9—C8—C7	0.6 (3)
C9—C4—C3—C2	−178.36 (17)	C6—C7—C8—C9	1.2 (3)
C5—O1—C1—O2	179.85 (15)	O3—C7—C8—C9	−174.88 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O4^{i}	0.98 (3)	2.46 (3)	3.296 (2)	142.6 (19)
C6—H5···O1^{ii}	0.96 (3)	2.51 (3)	3.444 (2)	167 (2)
C11—H11*A*···O2^{ii}	1.03 (3)	2.60 (3)	3.245 (2)	120.5 (18)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) −*x*+1, −*y*, −*z*+1.