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3-Butyl-1*H*-isochromen-1-one

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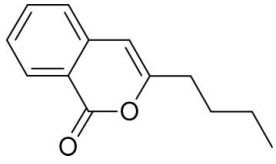
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.101; data-to-parameter ratio = 11.3.

In the title compound, $C_{13}H_{14}O_2$, a derivative of isocoumarin, the packing is stabilized by intermolecular C—H···O interactions.

Related literature

For related literature, see: Saeed *et al.* (2006, 2007). For background, see: Barry (1964) and Napolitano (1997).



Experimental

Crystal data

$C_{13}H_{14}O_2$
M_r = 202.24
Monoclinic, $P2_1/c$
a = 8.3929 (12) Å
b = 14.862 (2) Å
c = 8.8880 (12) Å
β = 95.963 (2)°
V = 1102.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 290 (2) K
0.47 × 0.42 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.927, T_{max} = 0.976
8442 measured reflections
2161 independent reflections
1201 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.101
S = 0.93
2161 reflections
192 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^{i}	0.952 (18)	2.584 (18)	3.363 (2)	139.2 (13)
C5—H5···O1^{ii}	0.949 (19)	2.496 (19)	3.397 (2)	158.5 (13)

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2496).

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supplementary materials

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3-Butyl-1*H*-isochromen-1-one

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Comment

Compounds containing the isocoumarin moiety show strong antifungal, antibacterial activity and are commonly found in higher plants,marine organisms and in variety of fungi,lichens and bacteria (Barry, 1964, Napolitano, 1997).

The structure of the title compound, (I) (Fig. 1), contains an *n*-butyl unit attached to the isocoumarin frame at the carbon atom C9.T he angle between the isocoumarin moiety and the n butyl side chain is 0.67° indicating that the entire molecule is almost planar. The *n*-butyl group adopts an all *trans* configuration.

The packing for (I) (Fig. 2) is consolidated by C—H···O interactions (Table 1).

Experimental

The title compound was synthesized from a mixture of homophthalic acid (1 mmol) and pentanoyl chloride (4 mmol)·The mixture was placed in a glass tube fitted with a tightened rubber septum and was refluxed at 393 K under a nitrogen atmosphere. The completion of the reaction was monitored by TLC using a hexane:ethylacetate (9:1 *v*/*v*) mixture. After the completion of reaction, the mixture was dissolved in dichloromethane and adsorbed on silica gel. The compound was purified by column chromatography using a mixture of hexane/ethyl acetate (9:1 *v*/*v*). Colourless blocks of (I) were recrystalized from ether.

Refinement

All the H atoms were located and refined isotropically resulting in C—H bond lengths of 0.93 (3)–1.02 (3) Å.

Figures

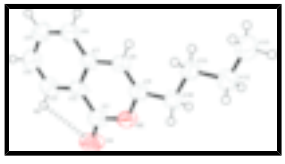

Fig. 1. View of the molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

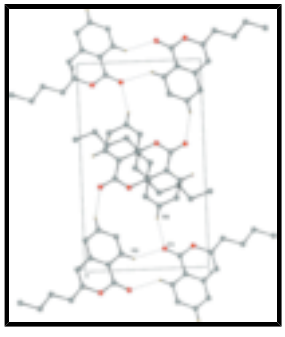

Fig. 2. Packing diagram of (I) viewed down the *a* axis. The dotted lines indicate intermolecular C—H···O interactions.

3-Butyl-1*H*-isochromen-1-one

Crystal data

$C_{13}H_{14}O_2$	$F_{000} = 432$
$M_r = 202.24$	$D_x = 1.218$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1190 reflections
$a = 8.3929$ (12) Å	$\theta = 2.5$–24.4°
$b = 14.862$ (2) Å	$\mu = 0.08$ mm^{-1}
$c = 8.8880$ (12) Å	$T = 290$ (2) K
$\beta = 95.963$ (2)°	Block, colourless
$V = 1102.6$ (3) Å^3	0.47 × 0.42 × 0.30 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2161 independent reflections
Radiation source: fine-focus sealed tube	1201 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.040$
$T = 290$(2) K	$\theta_{max} = 26.0^\circ$
φ and ω scans	$\theta_{min} = 2.4^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{min} = 0.927$, $T_{max} = 0.976$	$k = -18 \rightarrow 16$
8442 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.93$	$(\Delta/\sigma)_{max} < 0.001$
2161 reflections	$\Delta\rho_{max} = 0.14$ e Å^{-3}
192 parameters	$\Delta\rho_{min} = -0.14$ 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.16015 (18)	0.09619 (8)	−0.34990 (14)	0.0868 (5)
O2	0.27788 (14)	0.10418 (7)	−0.11803 (13)	0.0600 (4)
C1	0.1839 (2)	0.05878 (12)	−0.2290 (2)	0.0596 (5)
C2	0.12493 (18)	−0.02983 (11)	−0.19035 (17)	0.0492 (4)
C3	0.0271 (2)	−0.07876 (14)	−0.2979 (2)	0.0599 (5)
C4	−0.0265 (2)	−0.16201 (14)	−0.2621 (2)	0.0628 (5)
C5	0.0146 (2)	−0.19757 (14)	−0.1198 (2)	0.0622 (5)
C6	0.1090 (2)	−0.15013 (12)	−0.0126 (2)	0.0573 (5)
C7	0.16625 (18)	−0.06484 (10)	−0.04574 (17)	0.0457 (4)
C8	0.2651 (2)	−0.01165 (11)	0.06149 (19)	0.0511 (4)
C9	0.31617 (19)	0.06910 (11)	0.02615 (18)	0.0501 (4)
C10	0.4163 (2)	0.13379 (13)	0.1222 (2)	0.0567 (5)
C11	0.4656 (2)	0.10221 (13)	0.2824 (2)	0.0575 (5)
C12	0.5681 (3)	0.16981 (14)	0.3760 (2)	0.0677 (6)
C13	0.6172 (4)	0.13693 (19)	0.5347 (3)	0.0868 (7)
H3	0.0023 (19)	−0.0544 (11)	−0.398 (2)	0.071 (5)*
H4	−0.0935 (19)	−0.1958 (11)	−0.3365 (17)	0.065 (5)*
H5	−0.024 (2)	−0.2557 (12)	−0.0998 (17)	0.073 (6)*
H6	0.1368 (19)	−0.1730 (11)	0.0846 (18)	0.063 (5)*
H8	0.2914 (16)	−0.0350 (10)	0.1603 (16)	0.052 (4)*
H10A	0.3558 (18)	0.1912 (11)	0.1235 (16)	0.061 (5)*
H10B	0.514 (2)	0.1494 (10)	0.0729 (17)	0.070 (5)*
H11A	0.370 (2)	0.0877 (10)	0.3357 (17)	0.063 (5)*
H11B	0.5267 (18)	0.0431 (11)	0.2821 (16)	0.062 (5)*
H12A	0.509 (2)	0.2228 (13)	0.3777 (19)	0.079 (6)*
H12B	0.662 (2)	0.1838 (12)	0.3201 (19)	0.081 (6)*
H13A	0.524 (3)	0.1253 (14)	0.587 (3)	0.116 (9)*
H13B	0.676 (3)	0.0771 (15)	0.535 (2)	0.106 (8)*
H13C	0.680 (2)	0.1827 (14)	0.593 (2)	0.091 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1246 (13)	0.0719 (9)	0.0602 (9)	0.0015 (8)	−0.0084 (8)	0.0199 (7)
O2	0.0741 (9)	0.0484 (7)	0.0573 (7)	0.0005 (6)	0.0059 (6)	0.0082 (6)
C1	0.0697 (13)	0.0549 (12)	0.0532 (11)	0.0105 (9)	0.0025 (9)	0.0017 (9)
C2	0.0501 (11)	0.0473 (11)	0.0502 (10)	0.0110 (8)	0.0055 (8)	−0.0014 (8)
C3	0.0623 (12)	0.0676 (14)	0.0493 (12)	0.0100 (10)	0.0035 (9)	−0.0040 (10)
C4	0.0615 (13)	0.0656 (14)	0.0605 (12)	−0.0002 (10)	0.0036 (10)	−0.0188 (11)
C5	0.0647 (13)	0.0522 (12)	0.0706 (13)	−0.0034 (10)	0.0102 (10)	−0.0076 (11)
C6	0.0650 (12)	0.0506 (12)	0.0558 (12)	−0.0003 (9)	0.0040 (9)	0.0029 (9)
C7	0.0450 (10)	0.0431 (10)	0.0490 (10)	0.0073 (8)	0.0054 (8)	−0.0013 (8)
C8	0.0572 (11)	0.0499 (11)	0.0457 (10)	0.0032 (9)	0.0034 (8)	0.0067 (8)
C9	0.0522 (11)	0.0480 (11)	0.0505 (10)	0.0050 (8)	0.0068 (8)	0.0015 (8)
C10	0.0556 (12)	0.0474 (11)	0.0674 (12)	0.0015 (10)	0.0077 (10)	−0.0006 (9)
C11	0.0537 (12)	0.0542 (12)	0.0641 (12)	−0.0035 (10)	0.0031 (10)	−0.0026 (9)
C12	0.0726 (15)	0.0592 (14)	0.0701 (14)	−0.0040 (12)	0.0012 (12)	−0.0074 (10)
C13	0.103 (2)	0.0798 (18)	0.0735 (16)	−0.0185 (17)	−0.0112 (15)	−0.0058 (13)

Geometric parameters (Å, °)

O1—C1	1.2079 (18)	C8—C9	1.323 (2)
O2—C1	1.374 (2)	C8—H8	0.949 (14)
O2—C9	1.3899 (18)	C9—C10	1.487 (2)
C1—C2	1.460 (2)	C10—C11	1.516 (2)
C2—C7	1.397 (2)	C10—H10A	0.994 (16)
C2—C3	1.398 (2)	C10—H10B	0.993 (17)
C3—C4	1.365 (2)	C11—C12	1.514 (3)
C3—H3	0.960 (17)	C11—H11A	0.996 (16)
C4—C5	1.381 (2)	C11—H11B	1.018 (16)
C4—H4	0.963 (16)	C12—C13	1.509 (3)
C5—C6	1.370 (2)	C12—H12A	0.934 (18)
C5—H5	0.947 (18)	C12—H12B	0.998 (19)
C6—C7	1.398 (2)	C13—H13A	0.97 (2)
C6—H6	0.935 (15)	C13—H13B	1.02 (2)
C7—C8	1.435 (2)	C13—H13C	0.97 (2)
C1—O2—C9	122.55 (13)	C8—C9—C10	128.90 (16)
O1—C1—O2	116.22 (16)	O2—C9—C10	110.46 (14)
O1—C1—C2	126.57 (17)	C9—C10—C11	114.96 (15)
O2—C1—C2	117.21 (15)	C9—C10—H10A	107.7 (9)
C7—C2—C3	120.52 (16)	C11—C10—H10A	110.2 (8)
C7—C2—C1	119.65 (15)	C9—C10—H10B	109.8 (9)
C3—C2—C1	119.83 (16)	C11—C10—H10B	109.3 (9)
C4—C3—C2	119.74 (18)	H10A—C10—H10B	104.4 (13)
C4—C3—H3	120.8 (10)	C12—C11—C10	113.25 (16)
C2—C3—H3	119.4 (10)	C12—C11—H11A	108.8 (9)
C3—C4—C5	120.2 (2)	C10—C11—H11A	111.1 (9)

C3—C4—H4	119.7 (9)	C12—C11—H11B	108.5 (9)
C5—C4—H4	120.1 (9)	C10—C11—H11B	110.7 (8)
C6—C5—C4	120.8 (2)	H11A—C11—H11B	104.2 (12)
C6—C5—H5	121.7 (10)	C13—C12—C11	112.52 (18)
C4—C5—H5	117.6 (10)	C13—C12—H12A	110.6 (11)
C5—C6—C7	120.44 (18)	C11—C12—H12A	107.2 (11)
C5—C6—H6	121.8 (10)	C13—C12—H12B	112.3 (10)
C7—C6—H6	117.8 (10)	C11—C12—H12B	107.4 (10)
C2—C7—C6	118.29 (16)	H12A—C12—H12B	106.5 (15)
C2—C7—C8	118.51 (15)	C12—C13—H13A	110.8 (14)
C6—C7—C8	123.20 (15)	C12—C13—H13B	111.5 (12)
C9—C8—C7	121.43 (16)	H13A—C13—H13B	105.1 (19)
C9—C8—H8	120.1 (9)	C12—C13—H13C	110.5 (11)
C7—C8—H8	118.4 (9)	H13A—C13—H13C	106.7 (17)
C8—C9—O2	120.64 (16)	H13B—C13—H13C	112.0 (17)
C9—O2—C1—O1	−179.52 (14)	C1—C2—C7—C8	0.5 (2)
C9—O2—C1—C2	−0.4 (2)	C5—C6—C7—C2	−0.1 (2)
O1—C1—C2—C7	178.47 (17)	C5—C6—C7—C8	179.83 (16)
O2—C1—C2—C7	−0.5 (2)	C2—C7—C8—C9	0.4 (2)
O1—C1—C2—C3	−1.8 (3)	C6—C7—C8—C9	−179.56 (15)
O2—C1—C2—C3	179.20 (14)	C7—C8—C9—O2	−1.4 (2)
C7—C2—C3—C4	−1.0 (2)	C7—C8—C9—C10	178.95 (16)
C1—C2—C3—C4	179.31 (15)	C1—O2—C9—C8	1.4 (2)
C2—C3—C4—C5	0.5 (3)	C1—O2—C9—C10	−178.86 (14)
C3—C4—C5—C6	0.2 (3)	C8—C9—C10—C11	−0.2 (3)
C4—C5—C6—C7	−0.3 (3)	O2—C9—C10—C11	−179.87 (15)
C3—C2—C7—C6	0.8 (2)	C9—C10—C11—C12	179.66 (18)
C1—C2—C7—C6	−179.50 (14)	C10—C11—C12—C13	−179.5 (2)
C3—C2—C7—C8	−179.17 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	0.952 (18)	2.584 (18)	3.363 (2)	139.2 (13)
C5—H5···O1^{ii}	0.949 (19)	2.496 (19)	3.397 (2)	158.5 (13)

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

Fig. 1

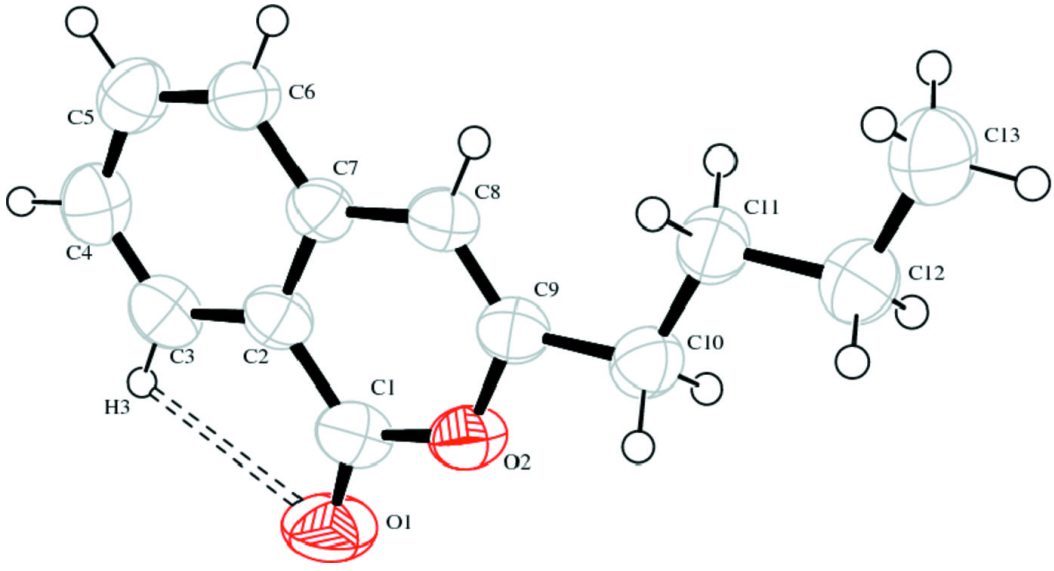

Fig. 2