intermolecular contact distances.* In this respect, the behaviour of the crystals of the title compound resembles that of the γ-modification of 2-*p*-dimethylaminobenzylidene-1,3-indandione (Magomeda, Zvonkova, Neigauz & Novakovskaya, 1980). In the α- and β-modifications, the intermolecular contacts are between dissimilar fragments leading to photosemiconductivity by electron charge transfer (Magmedova & Zvonkova, 1978, 1980).

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* See deposition footnote.

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Ethyl [3-(1,3-Dioxoindanylidene)-1-oxoindan-2-yl]acetate

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Abstract. $C_{22}H_{16}O_5$, $M_r = 360{\cdot}37$, monoclinic, $P2_1/n$, $a = 15{\cdot}857$ (5), $b = 6{\cdot}318$ (4), $c = 19{\cdot}667$ (5) Å, $\beta = 108{\cdot}89$ (2)°, $V = 1864{\cdot}2$ Å^3, $Z = 4$, $D_x = 1{\cdot}284$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 0{\cdot}54$ mm^{-1}, $F(000) = 752$, $T = 292$ K, $R = 0{\cdot}055$ for 2084 observed reflections. The C—O bond lengths in the ethoxycarbonylmethyl side chain indicate the presence of resonance structures of the carbonyl group. The molecule excluding the ethoxycarbonylmethyl side chain is essentially planar, while the side chain assumes an extended conformation.

Introduction. On account of the known biological activity of indan-1,3-dione and some of its derivatives, a number of structural studies of these compounds have been reported in recent years (*e.g.*, Csöregh & Eckstein, 1979, and references therein; Varghese, Srinivasan, Ramadas & Padmanabhan, 1986). The title compound is one of the new derivatives synthesized by Padmanabhan and Ramadas (Padmanabhan, 1982).

Experimental. Indan-1,3-dione on treatment with ethyl bromoacetate in the presence of freshly fused potassium carbonate in chloroform at room temperature gave a product containing two compounds. Column chromatography of this product on silica gel with benzene–hexane (2:1) furnished a new but unstable compound. The benzene eluates gave the stable title compound (m.p. 395 K). Recrystallization from ethanol gave shiny yellow needle-shaped crystals.

Crystal $0{\cdot}38 \times 0{\cdot}12 \times 0{\cdot}60$ mm, Enraf–Nonius CAD-4 diffractometer, graphite monochromator. Cell parameters refined by least-squares method on the basis of 25 reflections ($2 < 2\theta < 30°$). Two check reflections did not show significant variation during data collection. Lp correction, no absorption correction, no extinctions. 3279 reflections having $I > 3\sigma(I)$, $2 < 2\theta < 30°$, $h \pm 16$, $k \pm 7$, $l \pm 8$. Structure solved by

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multisolution direct methods using *MULTAN*80 (Main *et al.*, 1980) and difference Fourier syntheses using *SHELX*76 (Sheldrick, 1976). Final R factor with anisotropic thermal parameters except for H atoms is $R = 0{\cdot}0546$ (unit weights) and $wR = 0{\cdot}0539$ with $w = k[|\sigma(F_o)|^2 + g|F_o|^2]^{-1}$, where $k = 3{\cdot}7002$ and $g = 0{\cdot}002424$. The quantity minimized was $\sum w(|F_o| - k|F_c|)^2$. Refinement carried out with *SHELX*76 (Sheldrick, 1976). Max. $\Delta/\sigma = 0{\cdot}294$; max. and min. heights in final difference Fourier synthesis, 0·27 and $-0{\cdot}31\ \text{e}\ \text{Å}^{-3}$. Scattering factors from *SHELX*76.

Discussion. The final atomic coordinates are listed in Table 1* and an *ORTEP* (Johnson, 1965) plot of the molecule is shown in Fig. 1. Bond distances and bond angles are given in Table 2, and selected torsion angles in Fig. 2.

The $C(sp^2)$—$C(sp^2)$ bond lengths in the five-membered ring vary from 1·506 to 1·509 Å and equivalent bonds are equal within the limits of accuracy. However, the values of the lengths of corresponding bonds in different derivatives of indan-1,3-dione show remarkable variations [*e.g.*, 2-(2-nitrobenzylidene)indan-1,3-dione 1·474–1·487 Å (Varghese *et al.*, 1986)], reflecting varying degrees of resonance caused by chemical environments.

The expansion of the *ipso* angles and the contraction of the apical angles of the six-membered rings fused to small rings were as expected (Allen, 1981; Varghese *et al.*, 1986).

The significant difference in the lengths of the $C(sp^3)$—O and O—$C(sp^3)$ bonds, C(20)—O(5) [1·378 (4) Å] and O(5)—C(21) [1·481 (11) Å], is attributed to a partial contribution from the resonance structure $\text{O}^-\text{—C}{=}\text{O}^+\text{—C}$ for the group O(4)=C(20)—O(5)—C(21) (see Merlino, 1971). This feature, observed systematically in the carboxylic ester groups of substituents in various compounds, gives average values of 1·340 and 1·447 Å for these bonds. The bond angles involving the carbonyl O atom are invariably expanded (Dunitz & Schweizer, 1982).

The extended conformation of the side chain described by the torsion angles, τ[C(11)—C(19)—C(20)—O(5)] = −168·0 (6)° and τ[C(19)—C(20)—O(5)—C(21)] = 172·8 (6)°, in the title compound, is found to be the normal feature of the C—O—C—C terminal groups with alkyl substituents in many compounds (Dunitz & Schweizer, 1982).

Table 1. *Final fractional atomic coordinates* (× 10⁴ *for non-*H *atoms;* × 10³ *for* H *atoms*) *with e.s.d.'s in parentheses.*

$$U_{\text{eq}} = \sum_{i=1}^{3} U_{ii}/3.$$

	x	y	z	$U_{\text{eq}}(\times 10^3\ \text{Å}^2)$
C(1)	−277 (2)	−2542 (6)	3857 (2)	49 (2)
C(2)	85 (2)	−3566 (6)	3317 (2)	48 (2)
C(3)	−323 (2)	−2318 (6)	2637 (2)	55 (3)
C(4)	−1319 (2)	1164 (7)	2356 (2)	61 (3)
C(5)	−1764 (3)	2623 (8)	2644 (3)	65 (3)
C(6)	−1760 (3)	2441 (7)	3350 (2)	64 (3)
C(7)	−1293 (2)	800 (6)	3790 (2)	58 (2)
C(8)	−831 (2)	−663 (6)	3506 (2)	48 (2)
C(9)	−848 (2)	−508 (6)	2800 (2)	49 (2)
C(10)	632 (2)	−5328 (5)	3453 (2)	45 (2)
C(11)	959 (2)	−6426 (5)	4190 (2)	47 (2)
C(12)	1371 (2)	−8523 (6)	4061 (2)	52 (2)
C(13)	1719 (3)	−125 (7)	2984 (2)	65 (2)
C(14)	1672 (3)	−9811 (7)	2277 (2)	71 (2)
C(15)	1261 (3)	−7957 (8)	1920 (2)	74 (3)
C(16)	902 (3)	−6375 (8)	2246 (2)	64 (2)
C(17)	956 (2)	−6663 (6)	2960 (2)	47 (2)
C(18)	1366 (2)	−8548 (6)	3312 (2)	51 (2)
C(19)	1608 (2)	−5188 (6)	4818 (2)	48 (2)
C(20)	2470 (2)	−4636 (7)	4721 (2)	58 (3)
C(21)	3905 (6)	−8109 (20)	5330 (4)	175 (10)
C(22)	3986 (10)	−750 (21)	5300 (6)	288 (16)
O(1)	−165 (2)	−3131 (5)	4469 (1)	73 (2)
O(2)	−268 (2)	−2622 (6)	2043 (1)	88 (2)
O(3)	1659 (2)	−9934 (4)	4507 (1)	46 (2)
O(4)	2641 (2)	−4732 (5)	4177 (1)	76 (2)
O(5)	3043 (2)	−3969 (8)	5346 (1)	110 (3)
H(4)	−134 (2)	125 (6)	185 (2)	62 (14)
H(5)	−209 (3)	374 (9)	231 (3)	83 (18)
H(6)	−211 (3)	339 (8)	355 (3)	85 (16)
H(7)	−131 (2)	71 (6)	429 (2)	70 (11)
H(11)	48 (3)	680 (6)	435 (2)	72 (11)
H(13)	193 (3)	−140 (7)	322 (2)	76 (13)
H(14)	103 (3)	−1095 (7)	199 (2)	78 (13)
H(15)	126 (3)	−771 (6)	141 (2)	80 (12)
H(16)	64 (3)	−514 (7)	202 (2)	72 (15)
H(19*A*)	139 (2)	−384 (6)	490 (2)	50 (11)
H(19*B*)	170 (2)	−616 (5)	525 (2)	53 (8)
H(21*A*)	442 (4)	421 (6)	522 (4)	70 (9)
H(21*B*)	423 (5)	−328 (5)	599 (3)	72 (8)
H(22*A*)*	238	6	519	
H(22*B*)	434	−2	586	
H(22*C*)	425	−5	494	

* From H(22*A*) onwards atoms are geometrically fixed.

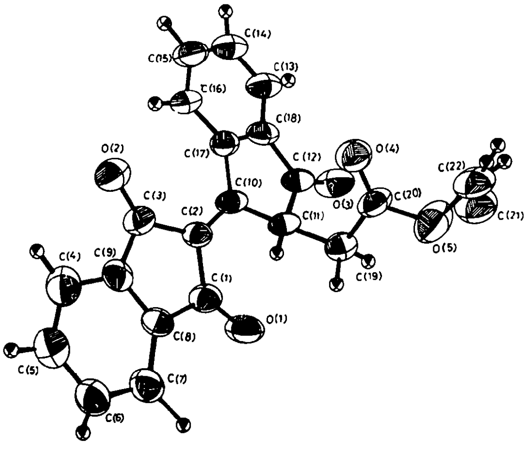

Fig. 1. *ORTEP* plot of the molecule showing thermal ellipsoids [O(2), O(5) at 70% probability; C(21), C(22) at 80% probability; other atoms at 50% probability].

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* Lists of structure factors, selected torsion angles, details of least-squares planes, intermolecular contact distances, bond lengths and angles involving H atoms, and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43082 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

C(1)—C(2)	1·507 (6)	C(12)—C(18)	1·471 (6)
C(2)—C(3)	1·506 (5)	C(18)—C(13)	1·399 (6)
C(3)—C(9)	1·509 (5)	C(13)—C(14)	1·383 (6)
C(9)—C(8)	1·383 (6)	C(14)—C(15)	1·412 (6)
C(8)—C(1)	1·506 (5)	C(15)—C(16)	1·404 (7)
C(1)—O(1)	1·217 (5)	C(16)—C(17)	1·391 (6)
C(3)—O(2)	1·215 (5)	C(17)—C(18)	1·424 (5)
C(9)—C(4)	1·419 (5)	C(10)—C(17)	1·496 (6)
C(4)—C(5)	1·388 (7)	C(11)—C(19)	1·541 (5)
C(5)—C(6)	1·391 (7)	C(12)—O(3)	1·230 (4)
C(6)—C(7)	1·399 (5)	C(19)—C(20)	1·482 (5)
C(7)—C(8)	1·403 (6)	C(20)—O(4)	1·187 (5)
C(2)—C(10)	1·383 (5)	C(20)—O(5)	1·338 (4)
C(10)—C(11)	1·538 (5)	C(21)—C(22)	1·499 (18)
C(11)—C(12)	1·535 (5)	C(21)—O(5)	1·481 (11)
C(1)—C(2)—C(3)	104·4 (3)	C(10)—C(11)—C(19)	117·4 (3)
C(1)—C(2)—C(10)	124·6 (3)	C(11)—C(10)—C(17)	106·0 (2)
C(2)—C(1)—C(8)	108·3 (3)	C(10)—C(17)—C(16)	131·2 (3)
C(1)—C(8)—C(7)	129·8 (3)	C(10)—C(17)—C(18)	108·1 (3)
C(1)—C(8)—C(9)	109·6 (3)	C(11)—C(12)—O(3)	126·0 (3)
C(2)—C(1)—O(1)	126·8 (3)	C(12)—C(11)—C(19)	111·2 (3)
C(8)—C(1)—O(1)	124·9 (3)	C(11)—C(19)—C(20)	114·9 (3)
C(2)—C(3)—C(9)	108·4 (3)	C(12)—C(18)—C(13)	126·6 (3)
C(3)—C(2)—C(10)	130·9 (3)	C(12)—C(18)—C(17)	109·4 (3)
C(2)—C(10)—C(11)	123·0 (3)	C(18)—C(12)—O(3)	125·9 (3)
C(2)—C(10)—C(17)	130·8 (3)	C(13)—C(14)—C(15)	119·0 (3)
C(3)—C(9)—C(4)	130·6 (3)	C(14)—C(13)—C(18)	117·5 (3)
C(3)—C(9)—C(8)	109·1 (3)	C(13)—C(18)—C(17)	124·0 (3)
C(9)—C(3)—O(2)	122·7 (3)	C(14)—C(15)—C(16)	123·6 (3)
C(4)—C(5)—C(6)	120·9 (4)	C(15)—C(16)—C(17)	117·8 (3)
C(5)—C(4)—C(9)	118·6 (3)	C(16)—C(17)—C(18)	118·0 (3)
C(4)—C(9)—C(8)	120·4 (3)	C(19)—C(20)—O(4)	126·4 (3)
C(5)—C(6)—C(7)	120·6 (3)	C(19)—C(20)—O(5)	109·7 (3)
C(6)—C(7)—C(8)	118·8 (3)	O(4)—C(20)—O(5)	124·0 (3)
C(7)—C(8)—C(9)	120·7 (3)	C(20)—O(5)—C(21)	116·9 (4)
C(10)—C(11)—C(12)	105·4 (2)	C(22)—C(21)—O(5)	117·2 (7)

The intermolecular contacts (C···O and C···C with minimum values of 3·21 and 3·53 Å, respectively) are van der Waals. Despite the O atoms of the carbonyl functions being involved in the intermolecular bonding, no dipolar bonds are found as in 2-dicyanomethyleneindan-1,3-dione (Silverman, Krukonis & Yannoni, 1974).

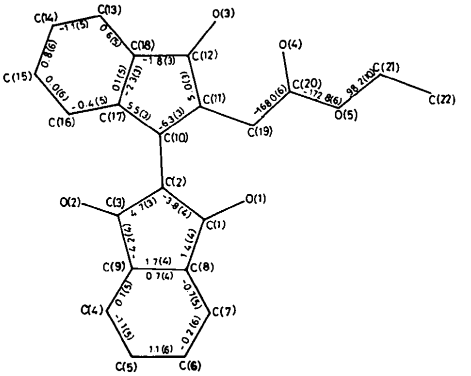

Fig. 2. Selected torsion angles (°) with e.s.d.'s in parentheses. τ[C(10)—C(11)—C(19)—C(20)] = −61·4 (4); τ[C(11)—C(19)—C(20)—O(4)] = 13·4 (5)°.

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2-(4-Oxo-2,3-diphenylindeno[1,2-*b*]pyrrol-1-yl)ethyl Acetate

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Abstract. $C_{27}H_{21}NO_3$, $M_r = 407{\cdot}469$, orthorhombic, $P2_12_12_1$, $a = 5{\cdot}823\ (2)$, $b = 14{\cdot}933\ (4)$, $c = 24{\cdot}067\ (3)$ Å, $V = 2092{\cdot}74$ Å^3, $Z = 4$, $D_x = 1{\cdot}293$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 0{\cdot}51$ mm^{-1}, $F(000) = 856$, $T = 293$ K, $R = 0{\cdot}043$ for 987 observed reflections. The C—O bond lengths in the β-acetylethyl side chain indicate the presence of resonance structures of the carbonyl group. The indenopyrrole fragment is

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