

## 4-(2-Indanoxy)phthalonitrile

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## Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$

$R$  factor = 0.049

$wR$  factor = 0.128

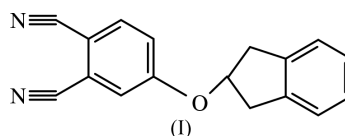
Data-to-parameter ratio = 19.9

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

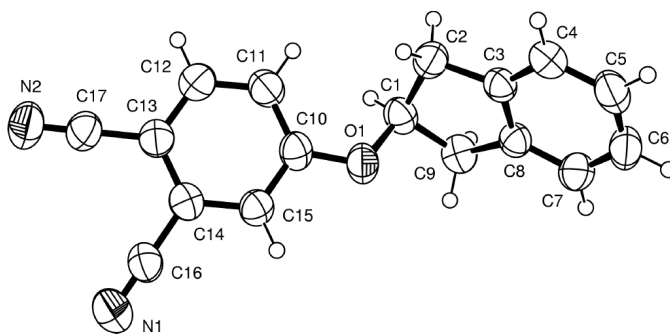
In the title molecule,  $\text{C}_{17}\text{H}_{12}\text{N}_2\text{O}$ , the five-membered ring of the indandione moiety adopts an envelope conformation. The dihedral angle between the 2-indanoxy and phthalonitrile groups, excluding the out-of-plane envelope flap atom, is  $59.81(5)^\circ$ .

## Comment

4-(2-Indanoxy)phthalonitrile, (I), is a precursor in the synthesis of peripherally tetra-substituted phthalocyanines (McKeown, 1998). Phthalocyanines are one of the major types of tetrapyrrole derivative, showing a wide range of applications in materials science, medicine and catalysis (Leznoff & Lever, 1989–1996).



The bonds lengths and angles in the phthalonitrile group are consistent with a previously published structure (Ocak *et al.*, 2003). The five-membered ring of the indanoxy group is in an envelope conformation, with atom C1 forming the flap (Fig. 1). Atoms C2/C3/C4/C5/C6/C7/C8/C9 are coplanar, with a maximum deviation of  $-0.018(2)\text{ \AA}$  for atom C9; atom C1 is  $0.351(2)\text{ \AA}$  from this plane. The bond lengths and angles in the five-membered ring in the title molecule are in agreement with expected values (Özbey *et al.*, 1995). The angle between the C10–C15 ring and the C2–C9 moiety is  $59.81(5)^\circ$ .



**Figure 1**

The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

## Experimental

2-Indanol (1 g, 7.75 mmol) was dissolved in dry dimethylformamide (30 ml) and 4-nitrophthalonitrile (1 g, 5.78 mmol) was added. After stirring for 30 min, finely ground anhydrous  $K_2CO_3$  (2 g, 14.50 mmol) was added portionwise over 2 h with vigorous stirring. The reaction mixture was stirred for 24 h at room temperature and then poured into ice-water (150 g). The product was filtered off and washed with water until the filtrate was neutral. Recrystallization twice from ethanol gave a green product. Yield 0.40 g (26.7%). Single crystals were obtained from absolute ethanol at room temperature *via* slow evaporation. M.p 403–405 K. Analysis, calcd: C: 78.44; H: 4.65; N: 10.76, found: C: 78.20; H: 4.70; N: 10.70%. IR data ( $\nu_{max}$ ,  $cm^{-1}$ ): 3080, 3020 (Ar–CH), 2920, 2850 (C–H), 2220 (C–N).

## Crystal data

$C_{17}H_{12}N_2O$   
 $M_r = 260.30$   
 Monoclinic,  $P2_1/a$   
 $a = 8.4711$  (8) Å  
 $b = 13.4082$  (8) Å  
 $c = 11.8736$  (11) Å  
 $\beta = 99.056$  (8)°  
 $V = 1331.82$  (19) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.298$  Mg  $m^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 12001 reflections  
 $\theta = 1.7–0.0^\circ$   
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Plate, colourless  
 $0.80 \times 0.43 \times 0.08$  mm

## Data collection

Stoe IPDS 2 diffractometer  
 $\varphi$  scans  
 Absorption correction: by integration *X-RED32* (Stoe & Cie, 2002)  
 $T_{min} = 0.916$ ,  $T_{max} = 0.992$   
 3702 measured reflections

3702 independent reflections  
 1467 reflections with  $I > 2\sigma(I)$   
 $\theta_{max} = 29.6^\circ$   
 $h = -11 \rightarrow 11$   
 $k = -18 \rightarrow 18$   
 $l = -16 \rightarrow 16$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.049$   
 $wR(F^2) = 0.128$   
 $S = 0.64$   
 3702 reflections  
 186 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0899P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.25$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.22$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXL97* (Sheldrick, 1997)  
 Extinction coefficient: 0.040 (3)

Table 1

Selected geometric parameters (Å, °).

O1–C10	1.358 (2)	C16–N1	1.137 (2)
O1–C1	1.452 (2)	C9–C1	1.519 (2)
C3–C8	1.388 (2)	C1–C2	1.525 (2)
C3–C2	1.497 (2)	C17–N2	1.139 (2)
C8–C9	1.495 (2)		
C10–O1–C1	118.34 (13)	C8–C7–C6	118.65 (17)
C6–C5–C4	120.53 (19)	C5–C6–C7	121.00 (18)

Atom H1 was located in a difference Fourier map and refined independently, with isotropic displacement parameters [ $C1–H1 = 0.961$  (18) Å]. The remaining H atoms were placed in calculated positions, with  $C(sp^2)–H$  distances of 0.93 Å and  $C(sp^3)–H$  distances of 0.97 Å. They were included in the refinement in the riding-model approximation, with  $U_{iso} = 1.2U_{eq}$  of the carrier atom. The intensity data collected for the title structure are generally weak, with only 40% having  $I > 2\sigma(I)$  for a maximum  $\theta$  angle of 29.5°.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999), *PARST* (Nardelli, 1995).

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