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Propyl 4-(3,4-dicyanophenoxy)benzoate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.061
wR factor = 0.153
Data-to-parameter ratio = 13.0

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

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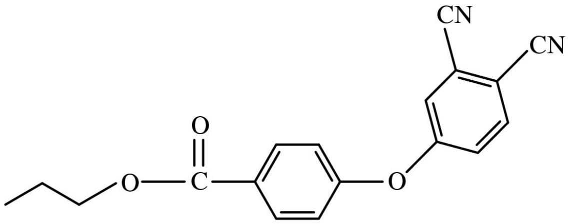
The title compound, $C_{18}H_{14}N_2O_3$, a phthalonitrile derivative, contains two aromatic rings, one of which carries two cyano groups. The crystal structure is stabilized by one intramolecular C—H···O and two intermolecular C—H···O hydrogen bonds.

Comment

Substituted phthalonitriles are generally used for preparing symmetrically and unsymmetrically peripherally substituted phthalocyanine complexes and subphthalocyanines (McKeown, 1998; Leznoff & Lever, 1989–1996). Around 80 000 tons per year of phthalocyanines are produced to be used as dyes and pigments (Wörhle, 2001). They are excellent pigments with good thermal and chemical stabilities and they have found wide applications in different fields, including liquid crystals, chemical sensors, photodynamic cancer therapy (Decreau *et al.*, 2001), non-linear optics, molecular electronics, gas sensors, photosensitisers, catalysts, semiconductive materials, photovoltaic cells and electrochromic displays (McKeown, 1998; Leznoff & Lever, 1989–1996).



(I)

Rings *A* (atoms C3–C8) and *B* (C9–C14) have a dihedral angle of 85.47 (11)°. The C≡N bond lengths (Table 1) display triple-bond character and are similar to values reported by Atalay *et al.* (2003) and Ocak, Çoruh *et al.* (2004).

The C—O bond lengths in the ester group agree with those of other esters (Bujak *et al.*, 2002; Ocak, Büyükgüngör *et al.*, 2004).

Experimental

Propyl 4-hydroxybenzoate (1.20 g, 6.66 mmol) and 4-nitrophthalonitrile (1.00 g, 5.78 mmol) were dissolved in dry dimethylformamide (30 ml) with stirring under N_2. Dry fine-powdered potassium carbonate (1.0 g, 7.24 mmol) was added in portions (10 × 1 mmol) every 10 min. The reaction mixture was stirred for 48 h at room temperature and poured into ice–water (150 g). The product was filtered off and washed with (10% *w*/*w*) NaOH solution and water until the filtrate was neutral. Recrystallization from ethanol gave a white product (yield 0.84 g, 47.46%). Single crystals were obtained from absolute ethanol at room temperature by slow evaporation (m.p. 373 K). Elemental analysis calculated for $C_{18}H_{14}N_2O_3$: C 70.58, H 4.61, N 9.14%; found: C 70.46, H 4.52, N 9.18%. IR (ν_{max}, cm^{-1}): 3055–3022 (Ar-CH), 2960–2865 (CH), 2221 (CN); ^{1}H NMR (CDCl$_3$): δ 1.05 (3H, *t*, CH$_3$), 1.80 (2H, *m*, CH$_2$), 4.31 (2H, *t*, CH$_2$—O), 7.11–7.36 (3H, *m*, Ar), 7.75–7.86 (2H, *d*, Ar), 8.13–8.18 (2H, *d*, Ar); ^{13}C NMR (CDCl$_3$): δ 10.45 (CH$_3$), 22.07 (CH$_2$), 66.84 (C—O), 109.90, 114.65 (CN), 115.07 (CN), 117.93, 119.88, 122.12, 122.32, 132.30, 135.52, 157.47, 160.61, 165.42 (C═O).

Crystal data

$C_{18}H_{14}N_2O_3$
$M_r = 306.31$
Monoclinic, $P2_1/c$
$a = 5.0843$ (9) Å
$b = 29.440$ (5) Å
$c = 10.823$ (2) Å
$\beta = 92.419$ (16)°
$V = 1618.5$ (5) Å^3
$Z = 4$

$D_x = 1.257$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3195 reflections
$\theta = 1.4$–21.3°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Needle, colourless
0.80 × 0.35 × 0.09 mm

Data collection

Stoe *IPDS*-2 diffractometer
ω scans
Absorption correction: none
10 034 measured reflections
3009 independent reflections
868 reflections with $I > 2\sigma(I)$

$R_{int} = 0.096$
$\theta_{max} = 25.5°$
$h = -5 \rightarrow 6$
$k = -35 \rightarrow 35$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.153$
$S = 0.81$
3009 reflections
231 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0129 (17)

Table 1
Selected geometric parameters (Å, °).

O2—C15	1.204 (4)	N1—C1	1.148 (4)
O3—C15	1.293 (4)	N2—C2	1.146 (5)
O2—C15—O3	123.5 (4)	O2—C15—C12	123.9 (5)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O2	0.93	2.46	2.786 (5)	101
C5—H5···O2^{i}	0.93	2.47	3.345 (4)	157
C16A—H16*A*···O2^{ii}	0.97	2.57	3.41 (2)	145

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

H atoms were positioned geometrically and refined using a riding model, fixing the aromatic C—H distances at 0.93 Å, methylene C—H distances at 0.97 Å and methyl C—H distances at 0.96 Å, with $U_{iso}(H) = 1.2U_{eq}$ (1.5 for methyl groups) of the parent atom. Atoms C16, C17 and C18 of the propyl group show positional disorder. The site-occupation factors of the disordered atoms refined to 0.526 (17) and 0.474 (17).

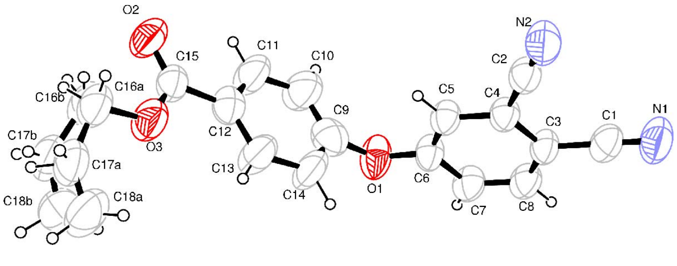


Figure 1
An *ORTEPIII* (Burnett & Johnson, 1996) drawing of the title compound, showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are drawn at the 30% probability level.

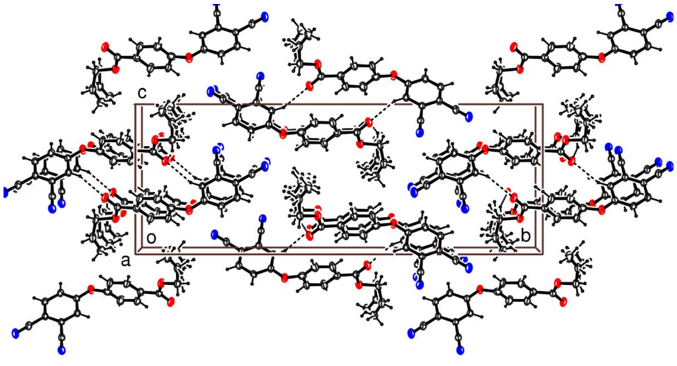


Figure 2
The packing of the title compound. Hydrogen bonds are shown as dashed lines.

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).

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