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4-(2,3-Dimethylphenoxy)phthalonitrile

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Key indicators

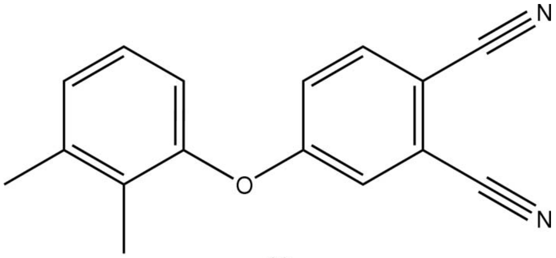
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.111
Data-to-parameter ratio = 15.1

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

In the title compound, $C_{16}H_{12}N_2O$, the planes of the 2,3-dimethylphenoxy group and phthalonitrile unit make a dihedral angle of 89.32 (4)°.

Comment

Substituted phthalonitriles are generally used for preparing symmetrically and unsymmetrically peripherally and non-peripherally substituted phthalocyanines and subphthalocyanines (McKeown, 1998; Leznoff & Lever, 1989–1996). In addition to their extensive use as dyes and pigments, phthalocyanines have found widespread applications in catalysis, in optical recording, as photoconductive materials, in photodynamic therapy and as chemical sensors (Leznoff & Lever, 1989–1996). We report here the crystal structure of the title phthalonitrile derivative, (I).



(I)

The molecular structure of compound (I) is shown in Fig. 1. The geometry of the phthalonitrile group agrees with those of previously reported structures (Janczak & Kubiak, 1995; Kartal *et al.*, 2006). The rings of the phthalonitrile unit and the 2,3-dimethylphenoxy group are both planar and they are twisted by a dihedral angle of 89.32 (4)°. The lengths of the two C—O bonds [C5—O1 = 1.3658 (15) Å and C9—O1 = 1.4092 (16) Å] are consistent with those found in similar compounds (Kartal *et al.*, 2006).

Experimental

Potassium carbonate (1.13 g, 8.19 mmol) was added to a solution of 2,3-dimethylphenol (0.5 g, 4.09 mmol) in dimethylformamide (50 ml). 4-Nitrophthalonitrile (0.7 g, 4.09 mmol) dissolved in dimethylformamide (50 ml) was then added. The mixture was stirred for 48 h at 298 K and poured into ice–water (150 g). The product was filtered off and washed with water. The product was recrystallized from ethanol to obtain solid 4-(2,3-dimethylphenoxy)phthalonitrile, (I). Crystals of (I) were obtained from a solution in ethanol at room temparature *via* slow evaporation (yield 51%, m.p. 392–394 K).

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Crystal data

$C_{16}H_{12}N_2O$
$M_r = 248.28$
Monoclinic, $C2/c$
$a = 13.7432$ (9) Å
$b = 9.3259$ (5) Å
$c = 21.0744$ (15) Å
$\beta = 94.476$ (6)°
$V = 2692.8$ (3) Å^3

$Z = 8$
$D_x = 1.225$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.63 × 0.54 × 0.38 mm

Data collection

Stoe IPDS 2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.901$, $T_{\max} = 0.984$

18971 measured reflections
2645 independent reflections
1989 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.029$
$\theta_{\max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.111$
$S = 1.05$
2645 reflections
175 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.229P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.12$ e Å^{-3}
$\Delta\rho_{\min} = -0.09$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0056 (8)

H atoms were included in calculated positions and treated using a riding model, with C—H(aromatic) = 0.93 Å and C(methyl)—H = 0.96 Å, and with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(parent C atom), or $1.5U_{\rm eq}$(methyl C atom).

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).

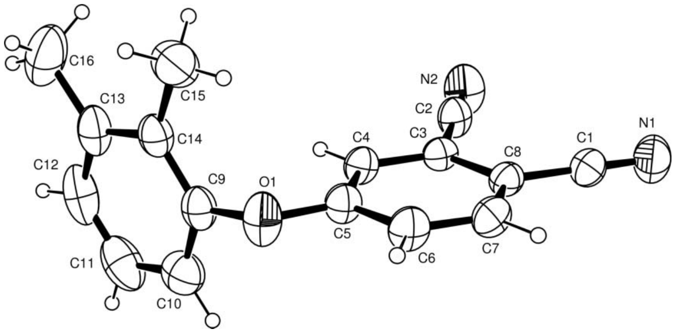

Figure 1
The molecular structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

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