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4-(*m*-Tolyloxy)phthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.102
Data-to-parameter ratio = 11.9

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

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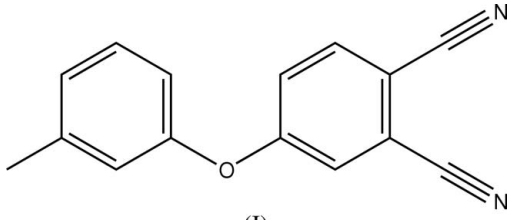
The crystal structure of the title phthalonitrile derivative, $C_{15}H_{10}N_2O$, is stabilized by π–π stacking interactions.

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 application in catalysis, in optical recording, as photoconductive materials, in photodynamic therapy and as chemical sensors (Leznoff & Lever, 1989–1996).



(I)

The geometry of the phthalonitrile group in the title compound, (I), agrees with that of previously reported structures (Janczak & Kubiak, 1995; Kartal *et al.*, 2006). The molecule is not planar, the dihedral angle between the phthalonitrile moiety and the *m*-tolyloxy group being 68.18 (4)°. The values of the two C—O bond lengths (Table 1) are consistent with those found in a similar compound (Kartal *et al.*, 2006).

In the crystal structure of (I) (Fig. 2), π–π stacking interactions are observed between the C3–C8 and C9–C14 aromatic rings of adjacent molecules, with a perpendicular interplanar distance of 3.7057 (10) Å and a centroid-to-centroid separation of 3.706 (2) Å.

Experimental

To a solution of 3-methylphenol (2.36 g, 21.8 mmol) in dimethylformamide (50 ml) were added potasium carbonate (6 g, 43.6 mmol) and a solution of 4-nitrophthalonitrile (3.77 g, 21.8 mmol) in dimethylformamide (50 ml). The mixture was stirred for 48 h at 298 K and then poured into ice–water (150 g). The product was filtered off, washed with water and recrystallized from ethanol to obtain solid 4-(*m*-tolyloxy)phthalonitrile. Crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature (yield 65%; m.p. 365–367 K).

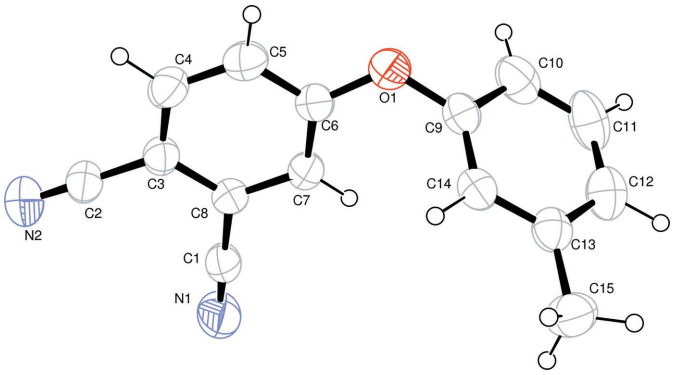


Figure 1
The molecular structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Crystal data

$C_{15}H_{10}N_2O$
M_r = 234.25
Monoclinic, $P2_1/c$
a = 11.5424 (8) Å
b = 8.5941 (5) Å
c = 14.4206 (11) Å
β = 120.223 (5)°
V = 1236.03 (16) Å^3
Z = 4
D_x = 1.259 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Prism, colourless
0.40 × 0.30 × 0.25 mm

Data collection

Stoe IPDS II diffractometer
ω scans
Absorption correction: none
15784 measured reflections
2434 independent reflections
1620 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.102
S = 1.02
2434 reflections
204 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.0394P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.011 (2)

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.1396 (19)	C6—O1	1.3583 (17)
C2—N2	1.138 (2)	C9—O1	1.3965 (18)
C6—O1—C9	120.71 (11)		

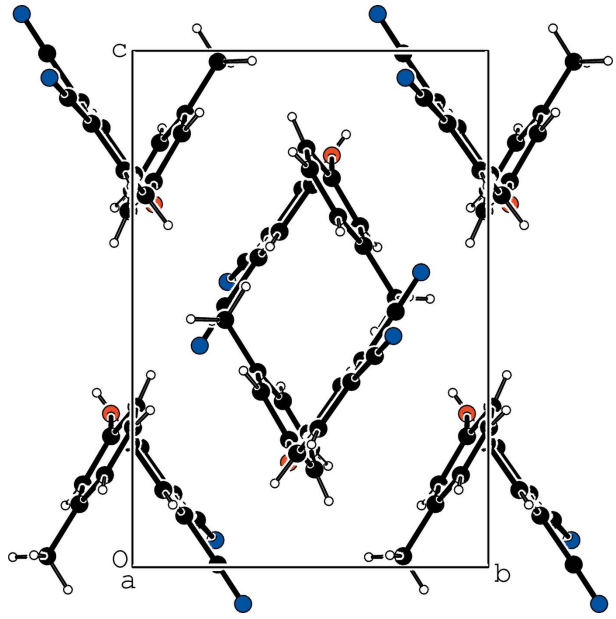


Figure 2
The crystal packing of (I), viewed down the *a* axis.

H atoms were found in a difference electron-density map and refined with isotropic displacement parameters. The range of C—H distances is 0.89 (2)–1.04 (2) Å.

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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