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4-(2-Methoxyphenoxy)phthalonitrile

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In the title compound, $C_{16}H_{12}N_2O_2$, the 2-methoxyphenoxy and phthalonitrile planes make a dihedral angle of 83.42 (7)°.

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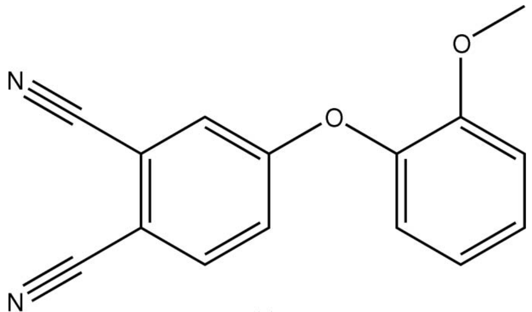
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.028
wR factor = 0.070
Data-to-parameter ratio = 8.5

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

Comment

Substituted phthalonitriles are generaly used in the preparation of symmetrically and unsymmetrically, peripherally and non-peripherally substituted phthalocyanines and sub-phthalocyanines (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, in 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 unit and the 2-methoxyphenoxy group is 83.42 (7)°. The lengths of the two C—O bonds [C6—O1 = 1.363 (2) and C9—O1 = 1.395 (2) Å] are consistent with those found in a similar compound (Kartal *et al.*, 2006).

Experimental

To a solution of 2-methoxyphenol (1.79 g, 14.4 mmol) in DMF (50 ml) was added potassium carbonate (4 g, 28.8 mmol). A solution of 4-nitrophthalonitrile (2.5 g, 14.4 mmol) in DMF (50 ml) was added. 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 then recrystallized from ethyl alcohol to obtain solid 4-(2-methoxyphenoxy)phthalonitrile. Crystals were obtained from ethanol at room temperature *via* slow evaporation (yield 62%, m.p. 384–386 K).

Crystal data

$C_{15}H_{10}N_2O_2$
$M_r = 250.25$
Orthorhombic, $P2_12_12_1$
$a = 7.790$ (6) Å
$b = 8.329$ (4) Å
$c = 19.575$ (12) Å
$V = 1270.0$ (14) Å^3

$Z = 4$
$D_x = 1.309$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
$0.55 \times 0.41 \times 0.29$ mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002) $T_{\min} = 0.971$, $T_{\max} = 0.982$

14897 measured reflections
1463 independent reflections
1223 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.044$
$\theta_{\max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.070$
$S = 1.01$
1463 reflections
173 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.10$ e Å^{-3}
$\Delta\rho_{\min} = -0.11$ e Å^{-3}

All H atoms were positioned geometrically and treated as riding, with C—H = 0.93 (aromatic) or 0.96Å (methyl) and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C) or $U_{\rm iso}$(H) = $1.5U_{\rm eq}$(methyl C). In the absence of significant anomalous scattering, Friedel pairs were merged.

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) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

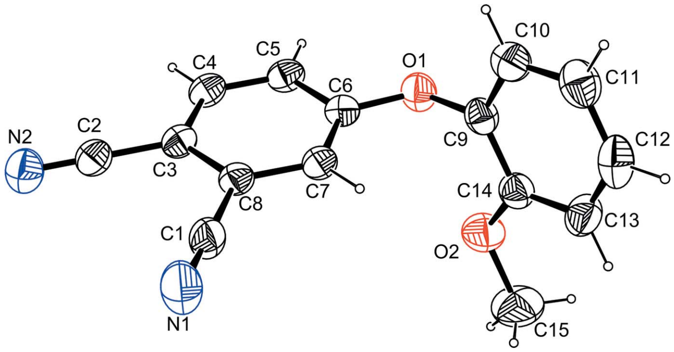


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radius.

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