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4-(2-Bromo-4-chlorophenoxy)phthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.057
wR factor = 0.144
Data-to-parameter ratio = 15.3

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

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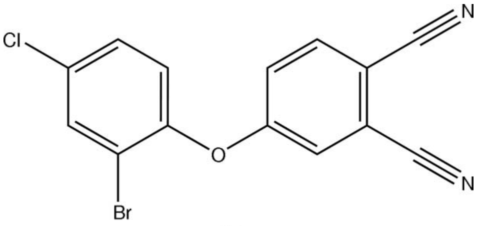
The title phthalonitrile derivative, $C_{14}H_6BrClN_2O$, contains two aromatic rings, which are almost perpendicular.

Comment

Substituted phthalonitriles are generally used for preparing symmetrically and unsymmetrically peripherally substituted phthalocyanine complexes and subphthalocyanines (McKeown, 1998; Leznoff & Lever, 1989–1996). Pthalocyanines possess some remarkable properties which render them important commercial commodities. In the last few years, a great deal of interest has been focused on the synthesis of phthalocyanine derivatives due to their applications in many fields, such as chemical sensors, electrochromism, batteries, semiconductive materials, liquid crystals, non-linear optics and photodynamic therapy (PDT) (Leznoff & Lever, 1989–1996).



(I)

An *ORTEPIII* (Burnett & Johnson, 1996) plot of the title compound, (I), is shown in Fig. 1. The lengths of the two C≡N triple bonds (Table 1) are consistent with those found in similar compounds (Atalay *et al.*, 2003; İskeleli & Ağar, 2005). The C—Br and C—Cl distances are close to the values reported for 4-(3-bromobenzylideneamino)-3-(4-chlorobenzyl)-4,5-dihydro-1*H*-1,2,4-triazol-5-one (Atalay *et al.*, 2004). The two aromatic rings in the molecule are almost perpendicular; the dihedral angle between ring A (atoms C3–C8) and ring B (atoms C9–C14) is 88.0 (3)°.

Experimental

2-Bromo-4-chlorophenol (1.40 g, 6.75 mmol) and 4-nitrophthalonitrile (1.1 g, 6.36 mmol) were dissolved in dry dimethylformamide (40 ml) with stirring under N_2 at 323 K. Dry fine-powdered potassium carbonate (2.0 g, 14.50 mmol) was added in portions (14 × 1 mmol) every 10 min. The reaction mixture was stirred for 48 h at 323 K and poured into ice–water (300 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 1.42 g, 73.96%). Single crystals were obtained from absolute ethanol at room temperature by slow evaporation (m.p. 407–408 K).

Crystal data

$C_{14}H_6BrClN_2O$
$M_r = 333.57$
Orthorhombic, *Pbca*
$a = 14.2841\ (14)$ Å
$b = 8.3753\ (5)$ Å
$c = 22.353\ (2)$ Å
$V = 2674.2\ (4)$ Å^3
$Z = 8$
$D_x = 1.657$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 21214 reflections
$\theta = 1.8$–$27.2°$
$\mu = 3.27$ mm^{-1}
$T = 293\ (2)$ K
Prism, colourless
$0.64 \times 0.34 \times 0.19$ mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.192$, $T_{\max} = 0.523$
22144 measured reflections
2634 independent reflections

1468 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.102$
$\theta_{\max} = 26.0°$
$h = -17 \rightarrow 17$
$k = -10 \rightarrow 10$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.144$
$S = 1.05$
2634 reflections
172 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 2.1953P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.79$ e Å^{-3}
$\Delta\rho_{\min} = -0.49$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C14	1.874 (7)	C5—O1	1.367 (6)
Cl1—C12	1.752 (6)	O1—C9	1.395 (7)
N1—C1	1.128 (6)	C2—N2	1.140 (7)
C5—O1—C9	119.2 (4)		

H atoms were positioned geometrically and treated using a riding model [atomatic C—H = 0.93 Å, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$].

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32*; 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).

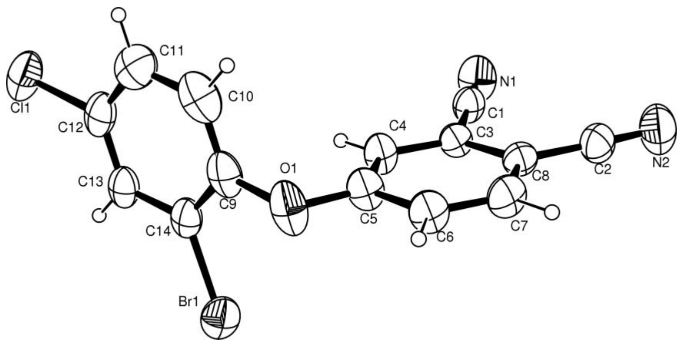


Figure 1
An *ORTEPIII* drawing (Burnett & Johnson, 1996) of the title compound showing the atomic numbering. Displacement ellipsoids of non-H atoms are drawn at the 20% probability level.

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