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3-[2-(2-Thienyl)ethoxy]phthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.071
wR factor = 0.244
Data-to-parameter ratio = 15.6

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

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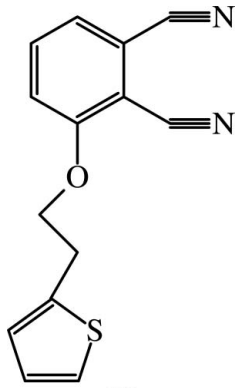
In the title compound, $C_{14}H_{10}N_2OS$, the thienyl and phthalonitrile planes make a dihedral angle of 57.92 (2)°.

Comment

Phthalocyanines have continuously been the subject of research due to their wide-ranging applications, such as organic pigments, chemical sensors, electrochromic display devices, photovoltaic cells, xerography, catalysis, non-linear optics and optical data storage, and also as carrier-generation materials in the near IR (Leznoff & Lever, 1993; McKeown, 1998).



(I)

The geometry of the phthalonitrile group in the title compound, (I), agrees with that of previously reported structures (Janczak & Kubiak, 1995; Tian *et al.*, 2002; Köysal *et al.*, 2003, 2004). The benzene and thienyl rings are both planar, with maximum deviations of 0.01 (3) Å for atom C12 and 0.01 (7) Å for atom C2, and they are twisted by a dihedral angle of 57.92 (2)°.

Experimental

2-(2-Thienyl)ethanol (1.00 g, 7.8 mmol) and 3-nitrophthalonitrile (1.35 g, 7.8 mmol) were dissolved in dry dimethyl sulfoxide (30 ml) with stirring under a nitrogen atmosphere. Dry fine-powdered potassium carbonate (5.38 g, 39 mmol) was added in portions every 10 min. The reaction mixture was stirred for 24 h at room temperature and poured into ice–water (200 g). The product was filtered off and washed with distilled water. Recrystallization from ethanol gave a white product (yield 1.23 g, 62%). Single crystals were obtained by slow evaporation of an absolute ethanol solution at room temperature (m.p. 377 K). Analysis calculated for $C_{14}H_{10}N_2OS$: C 66.12, H 3.96, N 11.02%; found: C 66.01, H 3.89, N 11.26%.

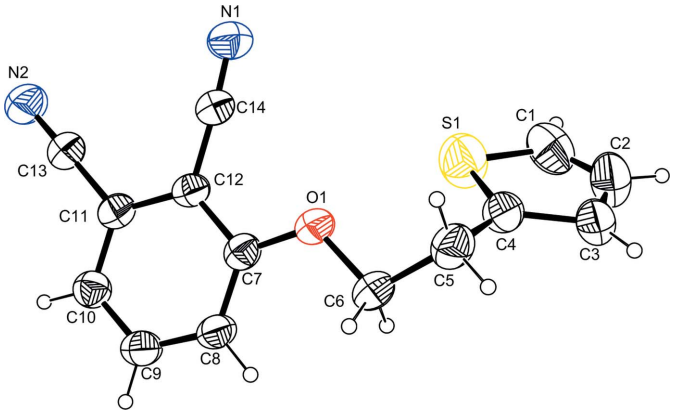


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

Crystal data

$C_{14}H_{10}N_2OS$
$M_r = 254.30$
Orthorhombic, *Pbca*
$a = 8.0888\ (4)$ Å
$b = 7.1356\ (4)$ Å
$c = 44.235\ (3)$ Å
$V = 2553.2\ (3)$ Å^3
$Z = 8$
$D_x = 1.323$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.24$ mm^{-1}
$T = 293\ (2)$ K
Plate, yellow
0.70 × 0.43 × 0.08 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.865$, $T_{max} = 0.982$
29377 measured reflections
2537 independent reflections
1370 reflections with $I > 2\sigma(I)$
$R_{int} = 0.074$
$\theta_{max} = 26.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.244$
$S = 0.95$
2537 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1655P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}

H atoms were positioned geometrically and refined using a riding model, with aromatic C—H = 0.93 Å, CH_2 C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

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) and *PARST* (Nardelli, 1995).

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