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2-Ethyl-5-nitroisoindoline-1,3-dione

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Key indicators

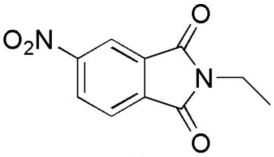
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.136
Data-to-parameter ratio = 14.1

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

In the title molecule, $C_{10}H_8N_20_4$, the phthalimide unit is essentially planar. In the crystal structure, weak intermolecular C—H···O hydrogen bonds link molecules into one-dimensional chains.

Comment

Phthalimides and *N*-substituted phthalimides are an important class of compounds because of their interesting biological activities (Lima *et al.*, 2002). The title compound, (I), is a precursor in the synthesis of *N*-substituted phthalimides and its crystal structure is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1. The phthalimide system is essentially planar to within 0.077 (3) Å. The geometry of the phthalimide system is comparable to that in the related crystal structures of 2-ethylisoindoline-1,3-dione (Liang *et al.*, 2006) and 5-amino-2-methylisoindoline-1,3-dione (Liang *et al.*, 2006). The dihedral angle between the nitro group plane and the phthalimide unit is 12.3 (2)°. In the crystal structure, weak intermolecular C—H···O hydrogen bonds link molecules into one-dimensional chains (Table 1 and Fig. 2).

Experimental

A mixture of 2-ethylisoindoline-1,3-dione (0.1 mol), nitric acid (0.11 mol) and sulfuric acid (0.55 mol) was kept at 353 K for 0.5 h.

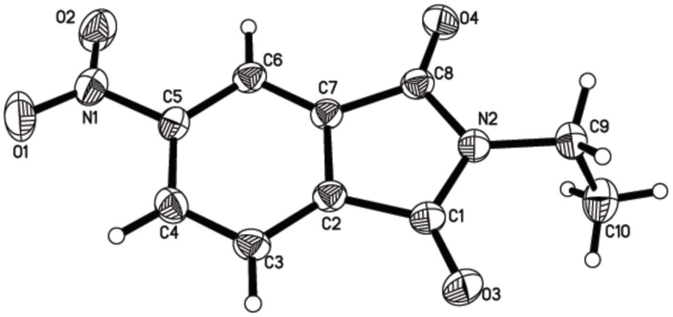


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

The mixture was then poured into cool water. After cooling, filtration, washing with water and drying, the title compound was obtained. 10 mg of (I) were dissolved in 10 ml acetic acid, and the solution was kept at room temperature for 15 d. Natural evaporation gave yellow single crystals of the title compound suitable for X-ray crystallographic analysis.

Crystal data

$C_{10}H_8N_2O_4$
$M_r = 220.18$
Orthorhombic, $P2_1/c$
$a = 4.9438$ (16) Å
$b = 20.655$ (6) Å
$c = 9.858$ (3) Å
$V = 1006.6$ (6) Å^3
$Z = 4$
$D_x = 1.453$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.12$ mm^{-1}
$T = 294$ (2) K
Block, yellow
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{\min} = 0.973$, $T_{\max} = 0.980$
5567 measured reflections
2058 independent reflections
1216 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.043$
$\theta_{\max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.136$
$S = 0.99$
2058 reflections
146 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 0.0778P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.19$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O3$^{\rm i}$	0.93	2.50	3.376 (2)	157
C3—H3···O4$^{\rm ii}$	0.93	2.40	3.314 (2)	167

Symmetry codes: (i) $x-1, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$.

H atoms were initially located in difference maps but were eventually placed in calculated positions and refined in the riding-model approximation, with C—H = 0.93–0.97 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or 1.5 $U_{\rm eq}$(methyl C).

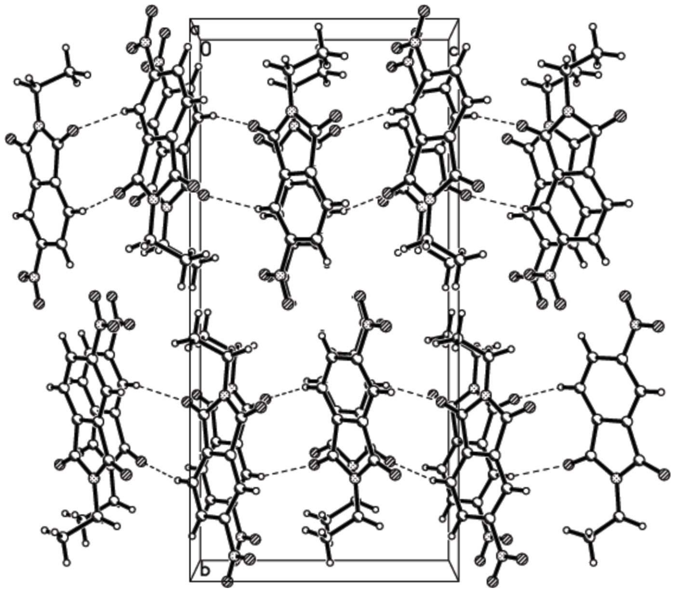


Figure 2
Part of the crystal structure of (I), showing hydrogen bonds as dashed lines.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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