Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Ethylisoindoline-1,3-dione

Zu-Pei Liang* and Jian Li

Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China

Correspondence e-mail: zupeiliang@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.045
wR factor = 0.113
Data-to-parameter ratio = 7.3

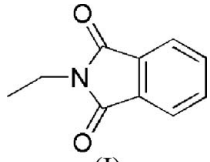
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 29 August 2006
Accepted 31 October 2006

The title compound, $C_{10}H_9NO_2$, was synthesized by mixing phthalic anhydride, ethanamine and triethylamine in toluene. The phthalimide unit is essentially planar. The crystal structure is stabilized by weak C—H···O hydrogen bonds.

Comment

Phthalimides and *N*-substituted phthalimides are an important class of compounds because of their interesting biological activities (Lima *et al.*, 2002; Orzeszka *et al.*, 2000; Bailleux *et al.*, 1993). Phthalimides have also served as starting materials and intermediates for syntheses of alkaloids (Couture *et al.*, 1998) and pharmacophores (Couture *et al.*, 1997). In this paper, the structure of the title compound, (I), is reported. The molecular structure of (I) is illustrated in Fig. 1.



(I)

The molecule has pseudo-mirror symmetry; the approximate mirror plane is perpendicular to the phthalimide ring system and passes through atoms N1, C9 and C10. The phthalimide unit is essentially planar, the maximum deviation from the mean plane passing through the atoms of the isoindoline ring (N1/C1–C8) being 0.013 (5) Å for atom C5. The geometry of the phthalimide ring system is close to that in the related compounds 4-(1,3-dioxoisoindolin-2-yl)benzaldehyde (Liu, *et al.*, 2004) and 5-amino-2-methylisoindoline-1,3-dione (Liang & Li, 2006).

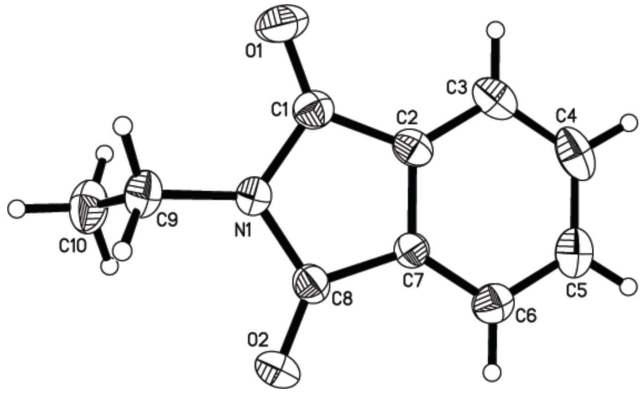


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

The crystal structure is stabilized by weak C—H···O hydrogen bonds (Fig. 2 and Table 1).

Experimental

A mixture of phthalic anhydride (0.1 mol), ethanolamine solution (65%) (0.13 mol) and triethylamine (0.01 mol) was stirred under reflux in toluene (30 ml) for 5 h. After cooling, filtration and drying, (I) was obtained. 10 mg of (I) were dissolved in 15 ml ethanol, and the solution was allowed to stand at room temperature. After 7 d, evaporation at room temperature gave colourless single crystals of the title compound.

Crystal data

$C_{10}H_9NO_2$
$M_r = 175.18$
Monoclinic, $P2_1$
$a = 7.254$ (6) Å
$b = 4.475$ (4) Å
$c = 13.506$ (10) Å
$\beta = 98.774$ (13)°
$V = 433.3$ (6) Å^3
$Z = 2$
$D_x = 1.343$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 294$ (2) K
Plate, colourless
0.32 × 0.26 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min} = 0.970$, $T_{max} = 0.981$
2113 measured reflections
866 independent reflections
617 reflections with $I > 2\sigma(I)$
$R_{int} = 0.071$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.113$
$S = 1.05$
866 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.0312P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O2^{i}	0.93	2.55	3.449 (6)	164

Symmetry code: (i) $x+1, y-1, z$.

All H atoms were located in difference Fourier maps. However, they were constrained in a riding-model approximation. The C—H distances were constrained to 0.93, 0.97 and 0.96 Å for the aryl, methylene and methyl H atoms, respectively, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). In the absence of significant anomalous dispersion effects, 630 Friedel pairs were merged prior to refinement.

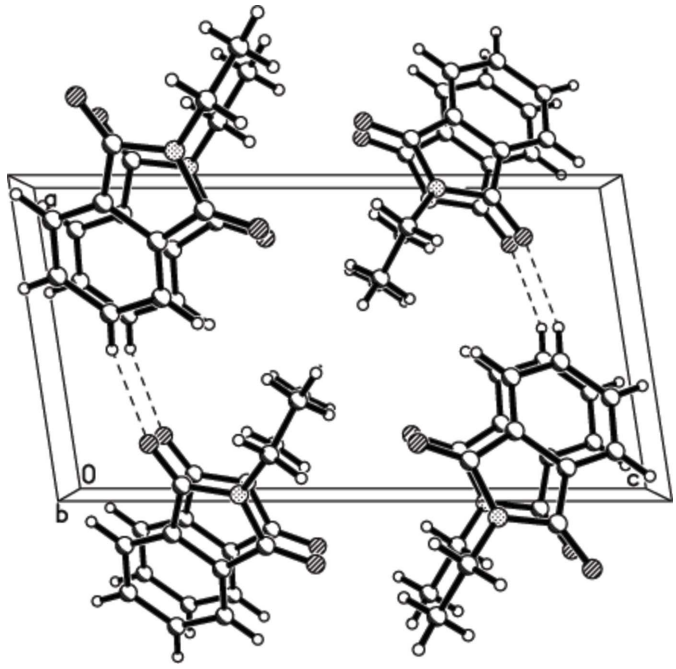


Figure 2
The crystal packing of (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

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*.

References

Bailleux, V., Vallee, L., Nuyts, J. P. & Vamecq, J. (1993). *Biomed. Pharmacother.* **47**, 463–464.
Bruker (1997). *SADABS*, *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Couture, A., Deniau, E., Grandclaudon, P. & Hoarau, C. (1998). *J. Org. Chem.* **63**, 3128–3132.
Couture, A., Deniau, E., Woisel, P. & Grandclaudon, P. (1997). *Synthesis (Stuttgart)*, **63**, 1439–1445.
Liang, Z.-P. & Li, J. (2006). *Acta Cryst.* E**62**, o4126–o4127.
Lima, L. M., Castro, P., Machado, A. L., Frage, C. A. M., Lugniur, C., Moraes, V. L. G. & Barreiro, E. (2002). *J. Biol. Org. Med. Chem.* **10**, 3067–3073.
Liu, X.-G., Feng, Y.-Q., Wu, P., Chen, X. & Li, F. (2004). *Acta Cryst.* E**60**, o2293–o2294.
Orzeszka, A., Kaminska, B., Orzeszko, G. & Starosciak, B. J. (2000). *Pharmacology*, **55**, 619–623.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.