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# 2-(2-Hydroxyethyl)isoindoline-1,3-dione

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In the title molecule, $C_{10}H_9NO_3$, the phthalimide unit is essentially planar and the hydroxyethyl substituent adopts a coiled conformation, with an N—C—C—O torsion angle of −65.3 (3)°. In the crystal structure, intermolecular O—H···O hydrogen bonds link molecules into one-dimensional chains along the *b*-axis direction.

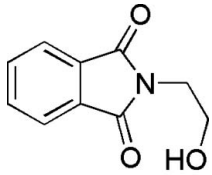
**Key indicators**

Single-crystal X-ray study
*T* = 294 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.043
*wR* factor = 0.112
Data-to-parameter ratio = 12.1

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

## Comment

*N*-Substituted phthalimides are an important class of compounds because of their interesting biological ctivities (Lima *et al.*, 2002). Phthalimides have also served as starting materials and intermediates for the syntheses of alkaloids and pharmacophores (Couture *et al.*, 1998). The molecular structure of the title compound, (I), is illustrated in Fig. 1. The phthalimide unit is planar to within 0.020 Å and the hydroxyethyl chain adopts a coiled conformation with an N1—C9—C10—O3 torsion angle of −65.6 (3)°. The geometry of the phthalimide ring system compares favourably with that in related compounds *e.g.* phthalimide 4-(1,3-dioxoisoindolin-2-yl)benzaldehyde (Liu *et al.*, 2004) and *N*-benzylphthalimide (Warzecha *et al.*, 2006).




(I)

In the crystal structure, intermolecular O—H···O hydrogen bonds link molecules into one-dimensional chains along the *b*-axis direction (Fig. 2 and Table 1).

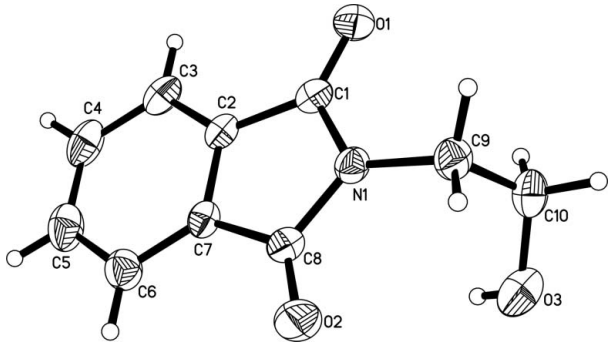



**Figure 1**
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

## Experimental

A mixture of phthalic anhydride (0.1 mol) and 2-aminoethanol (0.1 mol) was refluxed for 1.5 h. After cooling and filtration, the title compound was recrystallized from DMF (m.p. 401–403 K). 10 mg of (I) was dissolved in 15 ml ethyl acetate, The solution was allowed to evaporate at room temperature and colourless single crystals formed after 7 d.

*Crystal data*

$C_{10}H_9NO_3$
$M_r$ = 191.18
Monoclinic, $P2_1/n$
$a$ = 10.090 (4) Å
$b$ = 7.888 (3) Å
$c$ = 11.591 (4) Å
$\beta$ = 104.734 (6)°
$V$ = 892.2 (6) Å$^3$
$Z$ = 4
$D_x$ = 1.423 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 294 (2) K
Block, colourless
0.30 × 0.24 × 0.10 mm

*Data collection*

Bruker SMART CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min}$ = 0.969, $T_{max}$ = 0.989
3550 measured reflections
1566 independent reflections
962 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041
$\theta_{max}$ = 25.0°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.112
$S$ = 1.00
1566 reflections
129 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.0263P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.13 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.042 (5)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3···O1$^{i}$ | 0.82 | 2.07 | 2.869 (2) | 166 |

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

H atoms were positioned geometrically, with C—H = 0.93–0.97 Å and O—H = 0.82 Å. They were included in the refinement in the riding-model approximation, with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$($C_{methyl}$,O).

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) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

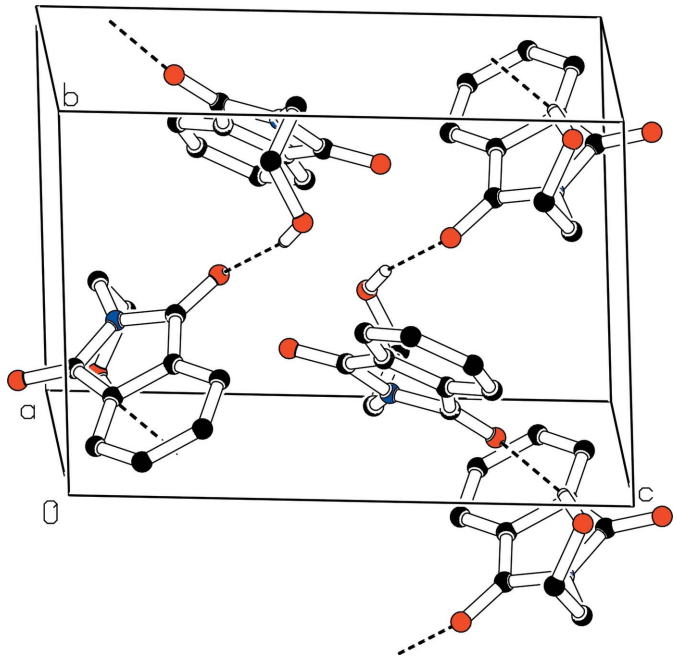



**Figure 2**
Part of the crystal structure of (I), with dashed lines indicating hydrogen bonds.

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