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2-(2-Iodoethyl)isoindole-1,3-dione

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Key indicators

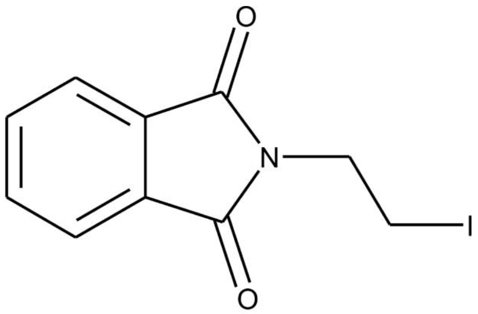
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.012 Å
R factor = 0.068
wR factor = 0.162
Data-to-parameter ratio = 18.6

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

The title compound, $C_{10}H_8INO_2$, is an *N*-substituted phthalimide derivative in which the crystallographic intermolecular contact pattern consists of I···I, C—H···I, C—H···O and aromatic π–π interactions.

Comment

The title compound, (I), is an *N*-substituted phthalimide (Fig. 1), whose crystal structure is stabilized by one I···I (Table 1) and one C—H···I (Table 2) intermolecular contact. There are also three intermolecular double C—H···O contact systems in the structure of (I) (Table 2). The first system is between C8 and O10, generating an $R_2^2(10)$ graph-set motif (Bernstein *et al.*, 1995). The two other systems are found between C13 and O11, with $R_2^2(12)$ motifs. One possible aromatic π–π stacking interaction is also found in the [010] direction, between a benzene ring at (x, y, z) and a diketopyrrole ring at (x, $1 + y$, z); the centroid-to-centroid distance is 3.911 (12) Å and the interplanar distance is 3.358 (14) Å.



(I)

Experimental

An excess of dry sodium iodide (2.6 g, 17 mmol) was mixed with *N*-(2-bromoethyl)phthalimide (1.1 g, 4 mmol) in dry acetone (100 ml). The resulting mixture was stirred at room temperature for 1 h and refluxed with stirring for an additional 2 h. It was then cooled to room temperature and evaporated to dryness. The residue was suspended in $CHCl_3$ and washed twice with water. The organic layer was dried with $MgSO_4$, filtered and evaporated. The residual oil was precipitated by addition of methanol and subsequent refrigeration. The product was crystallized from $CHCl_3$ after slow evaporation at room temperature, yielding colourless crystals (yield 0.43 g, 34%) suitable for X-ray analysis (m.p. 373 K). ^{1}H NMR (250 MHz, $CDCl_3$): δ 3.404 (*t*, 2H, H13*A* & *B*), 4.064 (*t*, 2H, H12*A* & *B*), 7.708–7.782 (*m*, 2H, H6 & H7), 7.841–7.915 (*m*, 2H, H5 & H8). GC–MS (EI): *m*/*z* (%) 301 (2.8).

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Crystal data

$C_{10}H_8INO_2$
$M_r = 301.07$
Monoclinic, $P2_1/n$
$a = 13.1099\ (11)$ Å
$b = 4.7775\ (2)$ Å
$c = 15.9655\ (14)$ Å
$\beta = 97.556\ (3)°$
$V = 991.28\ (13)$ Å^3
$Z = 4$
$D_x = 2.017$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.20$ mm^{-1}
$T = 173.0\ (1)$ K
Block, colourless
$0.30 \times 0.15 \times 0.07$ mm

Data collection

Bruker Kappa-APEX-II diffractometer
φ and ω scans
Absorption correction: multi-scan (*MULABS* in *PLATON*; Blessing, 1995; Spek, 2003)
$T_{\min} = 0.447$, $T_{\max} = 0.807$
4909 measured reflections
2357 independent reflections
1864 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.095$
$\theta_{\max} = 27.9°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.162$
$S = 1.09$
2357 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 15.0376P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.88$ e Å^{-3}
$\Delta\rho_{\min} = -1.45$ e Å^{-3}

Table 1
Selected contact distances (Å).

I14···I14$^{\rm i}$	3.8275 (9)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13B···O11$^{\rm ii}$	0.99	2.63	3.291 (10)	124
C13—H13A···O11$^{\rm iii}$	0.99	2.45	3.393 (11)	159
C8—H8···O10$^{\rm iv}$	0.95	2.43	3.344 (11)	161
C12—H12B···I14$^{\rm v}$	0.99	3.07	3.913 (8)	144

Symmetry codes: (ii) $-x+1, -y, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+2, -y, -z+1$; (v) $x, y-1, z$.

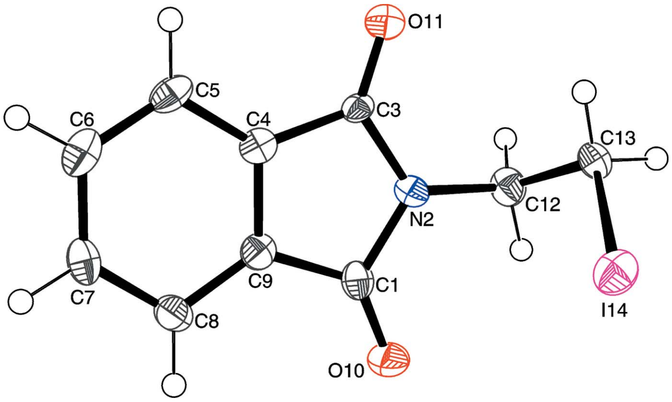

Figure 1
View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

All H atoms were visible in electron density maps, but were placed in idealized positions and allowed to ride on their parent atoms at C—H distances of 0.95 (aryl) and 0.99 Å (methylene), and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The deepest hole in the residual electron density lies 0.91 Å from I14.

Data collection: *COLLECT* (Bruker, 2004); cell refinement: *DENZO*–SMN (Otwinowski & Minor, 1997); data reduction: *DENZO*–SMN; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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