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2-[2,3-Bis(bromomethyl)-4-methoxyphenyl]-2,3-dihydro-1*H*-isoindole-1,3-dione

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In the title compound, $C_{17}H_{13}Br_2NO_3$, the dihedral angle between the benzene ring and the isoindole system is 71.3 (2)°. The crystal structure is stabilized by a C—H···O hydrogen bond and a π–π interaction.

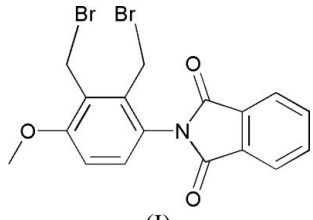
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.043
wR factor = 0.128
Data-to-parameter ratio = 16.9

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

Comment

Glycoluril derivatives have been studied extensively for a variety of purposes (Rowan *et al.*, 1999; Wu *et al.*, 2002). The title compound, (I), is an important intermediate in the synthesis of some glycoluril derivatives (Wu *et al.*, 2002).



(I)

The C2–C7 benzene ring is twisted with respect to the isoindole system, making a dihedral angle of 71.3 (2)° (Fig. 1). The crystal packing is consolidated by a C—H···O hydrogen bond (Table 1) and an intermolecular π–π stacking interaction between isoindole systems related by an inversion center (Fig. 2). The centroid–centroid and interplanar distances are 3.844 (3) and 3.613 (2) Å, respectively.

Experimental

The title compound was synthesized according to a literature procedure (Wu *et al.*, 2002). Single crystals suitable for X-ray analysis were grown from a dichloromethane solution at 277 K.

Crystal data

$C_{17}H_{13}Br_2NO_3$
M_r = 439.10
Triclinic, $P\overline{1}$
a = 8.7439 (11) Å
b = 8.7491 (12) Å
c = 11.0206 (15) Å
α = 83.426 (2)°
β = 86.704 (2)°
γ = 80.736 (2)°
V = 825.97 (19) Å^3
Z = 2
D_x = 1.766 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 4.92 mm^{-1}
T = 298 (2) K
Block, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.374, T_{max} = 0.374
6896 measured reflections
3536 independent reflections
2727 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.128$
$S = 1.11$
3536 reflections
209 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 0.0266P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.26$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1C···O2^{i}	0.96	2.44	3.225 (5)	139

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

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The highest residual electron-density peak is located 1.06 Å from atom Br2

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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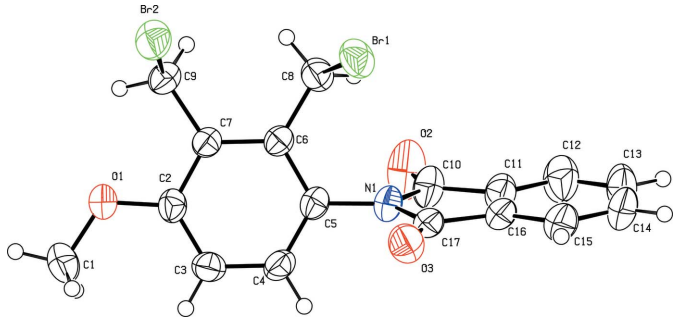

Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radius.

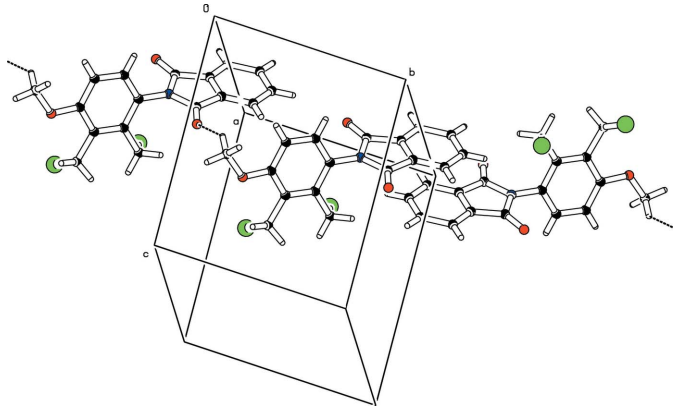

Figure 2
A partial packing diagram of (I), viewed approximately along the *a* axis. The dashed lines indicate C—H···O hydrogen bonds.

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