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## Key indicators

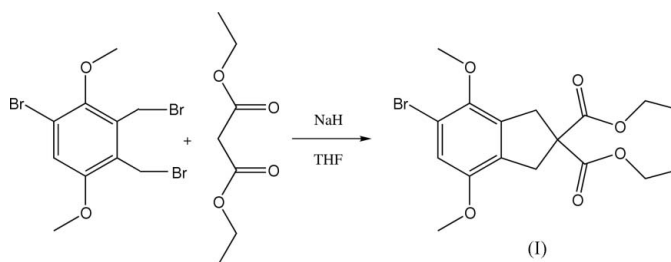
Single-crystal X-ray study  
 $T = 122$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.034  
 $wR$  factor = 0.081  
Data-to-parameter ratio = 31.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Diethyl 5-bromo-4,7-dimethoxyindan-2,2-  
dicarboxylate

The title compound,  $\text{C}_{17}\text{H}_{21}\text{BrO}_6$ , was prepared by nucleophilic alkylation of 1-bromo-3,4-bis(bromomethyl)-2,5-dimethoxybenzene. It crystallizes with two independent molecules in the asymmetric unit. The bond lengths and angles are generally within the normal ranges. The crystal packing is stabilized by weak intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds and weak  $\text{C}-\text{H}\cdots\pi(\text{arene})$  interactions.

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## Comment

The title compound, (I), was prepared for use as a building block in the syntheses of single-walled carbon nanotube (SWNT) interacting compounds. It crystallizes in the triclinic space group  $P\bar{1}$  with two independent molecules in the asymmetric unit (Fig. 1). The corresponding bond lengths and angles of the two molecules agree with each other, but the molecules differ in the orientations of the ester groups. In both molecules, one of the methoxy groups is coplanar with the benzene ring, while the other is almost perpendicular to the benzene ring (see torsion angles in Table 1) and the five-membered rings of the indan ring system adopt envelope conformations. The crystal packing of (I) is stabilized mainly by weak intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds and weak  $\text{C}-\text{H}\cdots\pi(\text{arene})$  interactions (Table 2 and Fig. 2).



## Experimental

1-Bromo-3,4-bis(bromomethyl)-2,5-dimethoxybenzene (50 g, 0.12 mol), prepared as described by Hammershøj *et al.* (2005), was dissolved in dried tetrahydrofuran (800 ml) and NaH (80% suspension in oil, 14 g) was added. The reaction mixture was stirred under an  $\text{N}_2$  atmosphere for 10 min at room temperature. Diethyl malonate (20 g, 0.2 mol) was dissolved in dried tetrahydrofuran (200 ml) and added over a 50 min period under an  $\text{N}_2$  atmosphere. After 2 h, brine (800 ml) was added and the mixture was extracted with diethyl ether ( $3 \times 200$  ml). The combined organic extracts were dried with  $\text{MgSO}_4$  and evaporated to dryness *in vacuo* yielding a pale green oil. Purification by crystallization in methanol yielded compound (I) as a white powder (30.2 g, 60%; m.p. 359–361 K);  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ):  $\delta$  6.6 (1H, s), 4.15 (4H, s,  $J$  7.14 Hz), 3.72 (3H, s), 3.7 (3H, s), 3.5 (2H, s), 3.4 (2H, s), 1.2 (6H, t);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  170.2, 151.1, 145.9, 134.0, 128.1, 113.6, 112.8, 60.8, 59.4, 54.7, 37.4, 36.6,

12.9; *m/e*: 402 (71), 328 (100), 253 (94), 69 (59.5) and 32 (87.5%); analysis calculated for  $C_{17}H_{21}BrO_6$ : C 50.89, H 5.28%; found: C 51.03, H 5.27%.

### Crystal data

$C_{17}H_{21}BrO_6$   
 $M_r = 401.24$   
 Triclinic,  $P\bar{1}$   
 $a = 11.1440$  (8) Å  
 $b = 11.1630$  (7) Å  
 $c = 15.7690$  (14) Å  
 $\alpha = 75.782$  (5)°  
 $\beta = 77.534$  (7)°  
 $\gamma = 73.395$  (5)°  
 $V = 1799.7$  (2) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.481$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 45017 reflections  
 $\theta = 1.4$ – $33.0$ °  
 $\mu = 2.31$  mm<sup>-1</sup>  
 $T = 122$  (2) K  
 Prism, white  
 $0.59 \times 0.34 \times 0.19$  mm

### Data collection

Nonius KappaCCD area-detector diffractometer  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: Gaussian integration (Coppens, 1970)  
 $T_{\min} = 0.427$ ,  $T_{\max} = 0.768$   
 72293 measured reflections  
 13426 independent reflections  
 11251 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.042$   
 $\theta_{\text{max}} = 33.0$ °  
 $h = -17 \rightarrow 17$   
 $k = -17 \rightarrow 16$   
 $l = -24 \rightarrow 24$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.081$   
 $S = 1.09$   
 13426 reflections  
 433 parameters  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 1.4569P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.002$   
 $\Delta\rho_{\text{max}} = 0.60$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.65$  e Å<sup>-3</sup>

**Table 1**

Selected torsion angles (°).

|                  |            |                  |            |
|------------------|------------|------------------|------------|
| C10A–O2A–C1A–C2A | –3.1 (2)   | C11B–O1B–C4B–C5B | 94.38 (15) |
| C10B–O2B–C1B–C2B | –2.13 (19) | C11A–O1A–C4A–C3A | 91.78 (18) |

**Table 2**

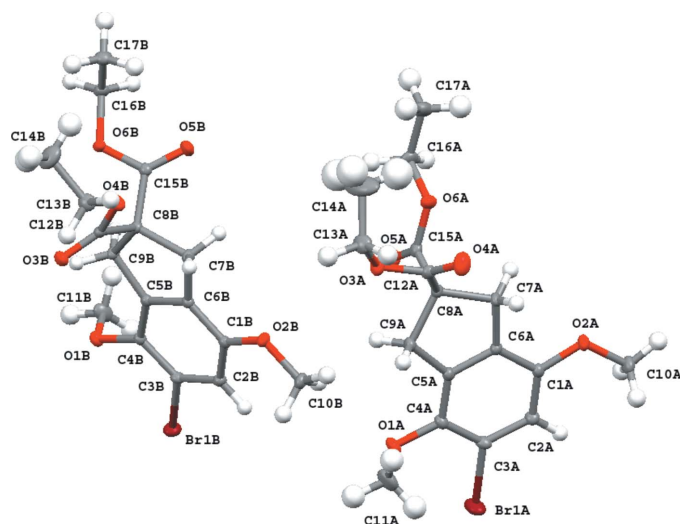
Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$                          | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| C7A–H7AB $\cdots$ O4A                  | 0.99  | 2.44        | 2.850 (2)   | 104           |
| C2A–H2A $\cdots$ O5A <sup>i</sup>      | 0.95  | 2.46        | 3.369 (2)   | 160           |
| C2B–H2B $\cdots$ O3B <sup>ii</sup>     | 0.95  | 2.56        | 3.419 (2)   | 150           |
| C13B–H13BB $\cdots$ O3B                | 0.99  | 2.36        | 2.717 (2)   | 100           |
| C9B–H9BA $\cdots$ O3B                  | 0.99  | 2.40        | 2.852 (2)   | 107           |
| C7B–H7BA $\cdots$ O5B                  | 0.99  | 2.38        | 2.849 (2)   | 108           |
| C9A–H9AB $\cdots$ O5A                  | 0.99  | 2.46        | 2.840 (2)   | 102           |
| C16A–H16AA $\cdots$ O3B <sup>iii</sup> | 0.99  | 2.57        | 3.260 (2)   | 127           |
| C10A–H10AA $\cdots$ O1B <sup>iv</sup>  | 0.98  | 2.55        | 3.462 (2)   | 155           |
| C10B–H10BA $\cdots$ O2A <sup>v</sup>   | 0.98  | 2.49        | 3.381 (2)   | 150           |
| C11B–H11BC $\cdots$ O5B <sup>iii</sup> | 0.98  | 2.57        | 3.427 (2)   | 146           |
| C17B–H17BC $\cdots$ O5A <sup>iii</sup> | 0.98  | 2.59        | 3.352 (2)   | 134           |
| C13A–H13AA $\cdots$ Cg1 <sup>v</sup>   | 0.99  | 2.82        | 3.799 (2)   | 171           |
| C16B–H16BB $\cdots$ Cg2 <sup>iii</sup> | 0.99  | 2.57        | 3.459 (2)   | 150           |

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

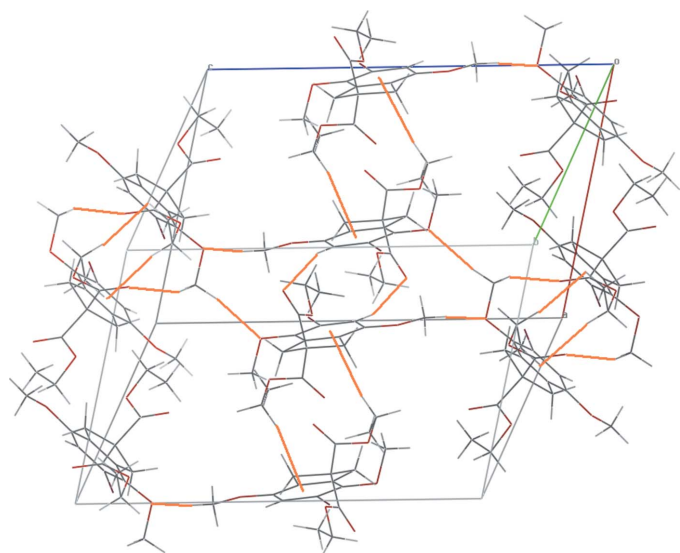
H atoms were placed in idealized positions and allowed to ride on their parent atoms, with  $C-H = 0.95$ – $0.99$  Å and  $U_{\text{iso}}(H) = 1.2$ – $1.5U_{\text{eq}}(C)$ .

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97*



**Figure 1**

The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.



**Figure 2**

The crystal packing of (I). C–H⋯O hydrogen bonds and C–H⋯ $\pi$ (arene) interactions are shown as brown lines.

(Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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