

## Dimethyl naphthalene-1,8-dicarboxylate

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## Key indicators

Single-crystal X-ray study

$T = 293$  K

Mean  $\sigma(\text{C}—\text{C}) = 0.009$  Å

$R$  factor = 0.051

$wR$  factor = 0.165

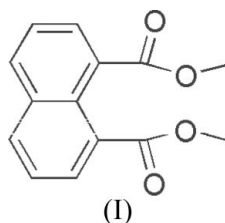
Data-to-parameter ratio = 7.2

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

In the title compound,  $\text{C}_{14}\text{H}_{12}\text{O}_4$ , the two ester groups are twisted away from the attached rings by  $43.9$  (2) and  $41.8$  (2)°. The crystal packing is stabilized by  $\text{C}—\text{H}\cdots\text{O}$  hydrogen bonds.

## Comment

1,8-Naphthalenedicarboxylic acid derivatives are a class of intermediates important for applications as monomers in the preparation of polymers (Nakayama *et al.*, 2001; Isoda & Yamada, 1995, 1996) or as sludge inhibitors (Raymond *et al.*, 1968). We report here the crystal structure of the title compound, (I).



The bond lengths and angles in (I) are normal (Table 1). The dihedral angle between the two aromatic rings of  $4.0$  (4)° indicates that the naphthalene ring system is slightly distorted from planarity. As a result of steric effects, the substituent groups at atoms C1 and C8 are twisted away from the plane of the naphthalene ring system (Fig. 1). The dihedral angle between the C1–C4/C9/C10 and O1/O2/C11/C12 planes is  $43.9$  (2)°, between the C5–C10 and O3/O4/C13/C14 planes is  $41.8$  (2)° and between the O1/O2/C11/C12 and O3/O4/C13/C14 planes is  $30.8$  (2)°. The crystal packing is stabilized by  $\text{C}—\text{H}\cdots\text{O}$  hydrogen bonds (Table 2).

## Experimental

Compound (I) was prepared according to the reported procedure of Louisa (1963). Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from methanol.

## Crystal data

$\text{C}_{14}\text{H}_{12}\text{O}_4$   
 $M_r = 244.24$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 5.9561$  (13) Å  
 $b = 12.043$  (5) Å  
 $c = 16.512$  (6) Å  
 $V = 1184.4$  (7) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.370$  Mg m<sup>−3</sup>

Mo  $K\alpha$  radiation  
 Cell parameters from 20 reflections  
 $\theta = 4.5–5.4^\circ$   
 $\mu = 0.10$  mm<sup>−1</sup>  
 $T = 293$  (2) K  
 Block, colourless  
 $0.30 \times 0.25 \times 0.23$  mm

### Data collection

Enraf–Nonius CAD-4  
diffractometer  
 $\omega/2\theta$  scans  
Absorption correction: none  
1343 measured reflections  
1183 independent reflections  
732 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.045$

$\theta_{\text{max}} = 25.0^\circ$   
 $h = 0 \rightarrow 7$   
 $k = 0 \rightarrow 14$   
 $l = 0 \rightarrow 19$   
3 standard reflections  
every 250 reflections  
intensity decay: none

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.051$   
 $wR(F^2) = 0.165$   
 $S = 1.10$   
1183 reflections  
165 parameters  
Only H-atom displacement  
parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0777P)^2 + 0.4255P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.26 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.29 \text{ e } \text{\AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O1—C11	1.330 (7)	O3—C14	1.437 (6)
O1—C12	1.441 (6)	O4—C13	1.199 (7)
O2—C11	1.206 (7)	C1—C11	1.505 (8)
O3—C13	1.365 (8)	C8—C13	1.489 (8)
C2—C1—C11	117.7 (5)	O2—C11—O1	124.8 (6)
C9—C1—C11	121.0 (5)	O2—C11—C1	124.5 (6)
C7—C8—C13	114.0 (5)	O4—C13—O3	123.3 (6)
C9—C8—C13	126.1 (6)	O4—C13—C8	126.1 (6)

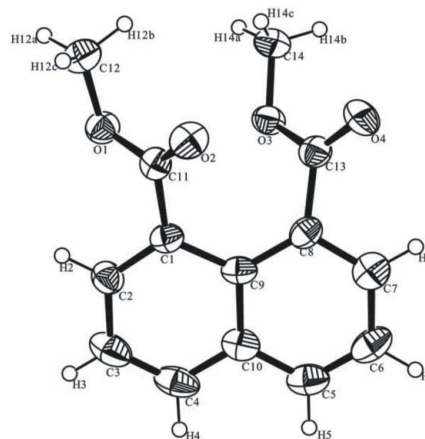
**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12A $\cdots$ O2 <sup>i</sup>	0.96	2.59	3.497 (9)	158
C14—H14A $\cdots$ O4 <sup>i</sup>	0.96	2.50	3.422 (9)	160
C4—H4 $\cdots$ O4 <sup>ii</sup>	0.93	2.56	3.489 (7)	173

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

The H atoms were placed in calculated positions, with C—H = 0.93 or 0.96  $\text{\AA}$ , and included in the final cycles of refinement using a riding model. A common displacement parameter was assigned separately for the aromatic and methyl H atoms and they were refined. In the absence of significant anomalous scattering effects, Friedel pairs were merged.



**Figure 1**

The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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