Dimethyl naphthalene-1,4-dicarboxylate

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Key indicators

Single-crystal X-ray study
$T = 291$ K
Mean σ(C–C) = 0.005 Å
R factor = 0.059
wR factor = 0.191
Data-to-parameter ratio = 11.0

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

In the title compound, $C_{14}H_{12}O_4$, the two ester groups are twisted away from the attached ring by 25.3 (3) and 14.6 (3)°. The crystal packing is stabilized by C—H···O hydrogen bonds.

Comment

1,4-Naphthalenedicarboxylic acid derivatives are a class of intermediates important for applications as monomers in the preparation of polymers (Fukuzumi *et al.*, 1994; Tsukada *et al.*, 1994) or printing receptors (Kuromya *et al.*, 1997). We report here the crystal structure of the title compound, (I).

(I)
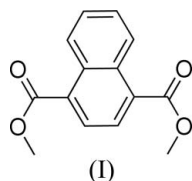
The bond lengths and angles in (I) are normal (Table 1). The naphthalene ring system is planar within 0.023 (3) Å. As a result of steric effects, the substituent groups at atoms C1 and C4 are twisted away from the plane of the naphthalene ring system (Fig. 1). The O1/O2/C11/C12 and O3/O4/C13/C14 planes form dihedral angles of 25.3 (3) and 14.6 (3)°, respectively, with the C1–C4/C9/C10 plane. The crystal packing is stabilized by C—H···O hydrogen bonds (Table 2).
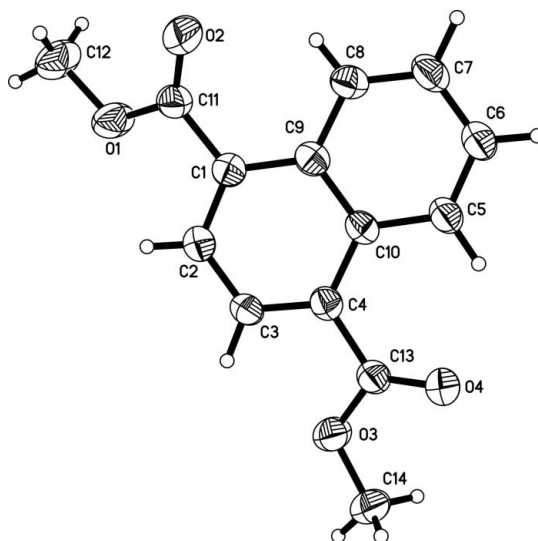
Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

Experimental

Compound (I) was prepared according to the reported precedure of Altunda & Balci (1993). Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from methanol.

Crystal data

$C_{14}H_{12}O_4$	$Z = 2$
$M_r = 244.24$	$D_x = 1.354$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.979$ (6) Å	Cell parameters from 18
$b = 9.222$ (4) Å	reflections
$c = 9.653$ (5) Å	$\theta = 4.5–7.4°$
$\alpha = 75.54$ (4)°	$\mu = 0.10$ mm^{-1}
$\beta = 69.18$ (5)°	$T = 291$ (2) K
$\gamma = 65.39$ (4)°	Block, colourless
$V = 599.3$ (7) Å^3	$0.25 \times 0.22 \times 0.22$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$\theta_{max} = 25.0°$
$\omega/2\theta$ scans	$h = -8 \rightarrow 9$
Absorption correction: none	$k = -7 \rightarrow 10$
2127 measured reflections	$l = -10 \rightarrow 11$
2087 independent reflections	3 standard reflections
1022 reflections with $I > 2\sigma(I)$	every 300 reflections
$R_{int} = 0.012$	intensity decay: 1.5%

Refinement

Refinement on F^2	H atoms treated by a mixture of
$R[F^2 > 2\sigma(F^2)] = 0.059$	independent and constrained
$wR(F^2) = 0.191$	refinement
$S = 0.94$	$w = 1/[\sigma^2(F_o^2) + (0.1139P)^2]$
2087 reflections	where $P = (F_o^2 + 2F_c^2)/3$
189 parameters	$(\Delta/\sigma)_{max} = 0.001$
	$\Delta\rho_{max} = 0.28$ e Å^{-3}
	$\Delta\rho_{min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C11	1.321 (4)	O3—C14	1.442 (4)
O1—C12	1.447 (4)	O4—C13	1.197 (4)
O2—C11	1.188 (4)	C1—C11	1.490 (4)
O3—C13	1.325 (4)	C4—C13	1.494 (4)
C11—O1—C12	116.6 (3)	O1—C11—C1	112.1 (3)
C13—O3—C14	117.9 (3)	O4—C13—O3	120.8 (3)
O2—C11—O1	121.6 (3)	O4—C13—C4	127.0 (3)
O2—C11—C1	126.3 (3)	O3—C13—C4	112.2 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1	0.90 (4)	2.33 (4)	2.688 (5)	104 (3)
C3—H3···O3	0.96 (4)	2.25 (3)	2.652 (5)	105 (3)
C5—H5···O4	0.99 (4)	2.15 (4)	2.879 (6)	128 (3)
C6—H6···O4^i	0.98 (5)	2.54 (5)	3.440 (6)	154 (3)
C7—H7···O2^{ii}	1.00 (4)	2.56 (3)	3.362 (6)	137 (2)
C8—H8···O2	0.89 (3)	2.23 (3)	2.891 (6)	130 (3)

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

Aromatic H atoms were located in a difference Fourier map and refined isotropically. The range of C—H bond lengths is 0.89 (3)–1.00 (3) Å. Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and included in the final cycles of refinement using a riding model [U_{iso}(H) = 1.5U_{eq}(C). A rotating group model was used for the methyl groups.

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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