

Diphenyl naphthalene-1,4-dicarboxylate

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Key indicators

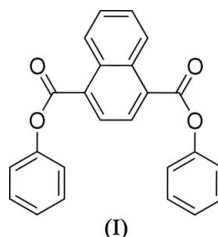
Single-crystal X-ray study
 $T = 292\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.047
 wR factor = 0.119
Data-to-parameter ratio = 10.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound, $\text{C}_{24}\text{H}_{16}\text{O}_4$, the two carboxylate groups are twisted away from the attached of the naphthalene unit ring by 20.4 (2) and 45.2 (1)° . The crystal packing is stabilized by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and $\text{C}-\text{H}\cdots\pi$ interactions.

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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 have recently reported the crystal structure of dimethyl naphthalene-1,4-dicarboxylate (Jing *et al.*, 2005). We report here the crystal structure of diphenyl naphthalene-1,4-dicarboxylate, (I).



The bond lengths and angles in (I) are normal (Table 1). The naphthalene ring system is planar within $0.033\text{ (2)}\text{ \AA}$. 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/C4/C11 and O3/O4/C1/C18 planes form dihedral angles of 20.4 (2) and 45.2 (1)° , respectively, with the C1–C4/C9/C10 plane. The dihedral angle between the O1/O2/C4/C11 and C12–C17 planes is 87.9 (1)° , and that between the O3/O4/C1/C18 and C19–C24 planes is 67.4 (1)° . The crystal packing is stabilized by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and $\text{C}-\text{H}\cdots\pi$ interactions involving the naphthalene ring system and the C12–C17 benzene ring (Table 2).

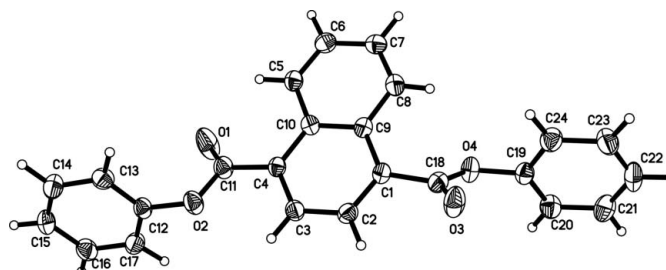


Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

Experimental

Compound (I) was prepared according to the reported procedure of Strey & Voss (1998). Brown single crystals suitable for X-ray diffraction study were obtained by recrystallization from dimethyl sulfoxide.

Crystal data

C₂₄H₁₆O₄ Z = 4
 M_r = 368.37 D_x = 1.360 Mg m⁻³
 Monoclinic, P2₁/c Mo Kα radiation
 a = 13.984 (7) Å μ = 0.09 mm⁻¹
 b = 5.7797 (17) Å T = 292 (2) K
 c = 22.283 (6) Å Block, brown
 β = 92.15 (3)° 0.30 × 0.30 × 0.23 mm
 V = 1799.7 (12) Å³

Data collection

Enraf–Nonius CAD-4 1324 reflections with I > 2σ(I)
 diffractometer R_{int} = 0.017
 ω/2θ scans θ_{max} = 25.4°
 Absorption correction: none 3 standard reflections
 3304 measured reflections every 300 reflections
 3280 independent reflections intensity decay: none

Refinement

Refinement on F² All H-atom parameters refined
 R[F² > 2σ(F²)] = 0.048 w = 1/[σ²(F_o²) + (0.0493P)²]
 wR(F²) = 0.119 where P = (F_o² + 2F_c²)/3
 S = 0.89 (Δ/σ)_{max} = 0.001
 3280 reflections Δρ_{max} = 0.18 e Å⁻³
 317 parameters Δρ_{min} = -0.19 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

O1–C11	1.179 (3)	O3–C18	1.188 (3)
O2–C11	1.346 (3)	O4–C18	1.363 (3)
O2–C12	1.407 (3)	O4–C19	1.404 (3)
C11–O2–C12	117.4 (2)	C17–C12–O2	118.4 (3)
C18–O4–C19	117.3 (2)	O3–C18–O4	122.6 (3)
O1–C11–O2	121.0 (3)	O3–C18–C1	124.9 (3)
O1–C11–C4	127.4 (3)	O4–C18–C1	112.4 (2)
O2–C11–C4	111.6 (3)	C20–C19–O4	118.3 (3)
C13–C12–O2	119.2 (3)	C24–C19–O4	119.9 (3)

Table 2

Hydrogen-bond geometry (Å, °).

D–H···A	D–H	H···A	D···A	D–H···A
C5–H5···O1	0.95 (2)	2.23 (2)	2.884 (4)	125 (2)
C5–H5···O1 ⁱ	0.95 (2)	2.60 (2)	3.264 (4)	128 (2)
C8–H8···O4	0.94 (2)	2.34 (2)	2.951 (4)	123 (2)
C2–H2···Cg1 ⁱⁱ	0.96 (3)	2.65 (3)	3.469 (4)	143 (2)
C6–H6···Cg2 ⁱ	0.99 (3)	2.76 (3)	3.596 (4)	142 (2)

Symmetry codes: (i) -x + 1, -y, -z + 2; (ii) -x + 1, y + 1/2, -z + 3/2. Cg1 and Cg2 are the centroids of the C1–C4/C9/C10 and C12–C17 benzene rings.

All H atoms were located in a difference Fourier map and refined isotropically. The range of C–H bond lengths is 0.92 (2)–1.01 (3) Å.

Data collection: *DIFRAC* (Gabe *et al.*, 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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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