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Diisopropyl anthracene-1,8-dicarboxylate

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In the title compound, $C_{22}H_{22}O_4$, the anthracene ring system is slightly non-planar. The two carboxylate groups are both twisted away from the plane of the anthracene ring system by *ca.* 30°. The crystal packing is stabilized by C—H⋯O hydrogen bonds.

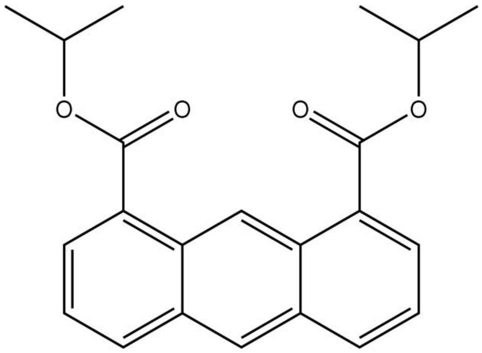
Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.001 Å
R factor = 0.033
wR factor = 0.101
Data-to-parameter ratio = 17.3

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

Comment

The photodimerization of anthracene and its derivatives has been extensively investigated in the fields of photochromic materials and the preservation of photoenergy (Grimme *et al.*, 1999; Sasaki *et al.*, 1992). The means of achieving controlled derivatives of anthracene has been described earlier (Tamaki *et al.*, 1987; Ueno *et al.*, 1991; Ueno *et al.*, 1989). We present here the crystal structure of the title anthracene derivative, (I).



(I)

Bond lengths and angles in (I) are normal. The anthracene ring system is slightly non-planar, with a maximum deviation of 0.074 (1)° for atom C6 from the least-squares plane. As a result of steric effects, the groups at atoms C1 and C8 are twisted away from the plane of the anthracene ring system (Fig. 1). The O1/O2/C15/C16 and O3/O4/C19/C20 planes form dihedral angles of 32.21 (1) and 28.30 (1)°, respectively, with the C1–C4/C11/C12 and C5–C8/C13/C14 planes

Experimental

Compound (I) was prepared by refluxing anthracene-1,8-dicarboxylic acid (2.9 g, 10 mmol) in propan-2-ol (400 ml) with concentrated sulfuric acid (4 ml) for 16 h. Water (100 ml) was added to the warm brown solution, and the product was extracted with dichloromethane. Concentration of the solvent by rotary evaporation left a brown oil, which was chromatographed (silica, dichloromethane) to yield the pure substance (yield 1.8 g, 61%). Yellow single crystals of (I) suitable for X-ray diffraction were obtained by recrystallization from ethyl acetate.

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Crystal data

$C_{22}H_{22}O_4$
$M_r = 350.40$
Monoclinic, $P2_1/c$
$a = 10.4097$ (2) Å
$b = 7.9541$ (1) Å
$c = 22.2260$ (4) Å
$\beta = 99.749$ (1)°
$V = 1813.73$ (5) Å^3

$Z = 4$
$D_x = 1.283$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 153$ (2) K
Block, yellow
0.45 × 0.43 × 0.41 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: none
17341 measured reflections

4161 independent reflections
3768 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.015$
$\theta_{\rm max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.101$
$S = 1.03$
4161 reflections
240 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.3998P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.30$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0079 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O3^{i}	1.00	2.55	3.440 (1)	149
C17—H17A···O4^{ii}	0.98	2.59	3.552 (1)	169
C21—H21A···O2^{ii}	0.98	2.55	3.492 (1)	162

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

All H atoms were placed in calculated positions and were included in the final cycles of refinement using a riding model, with C—H = 0.95–1.00 Å and with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C).

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

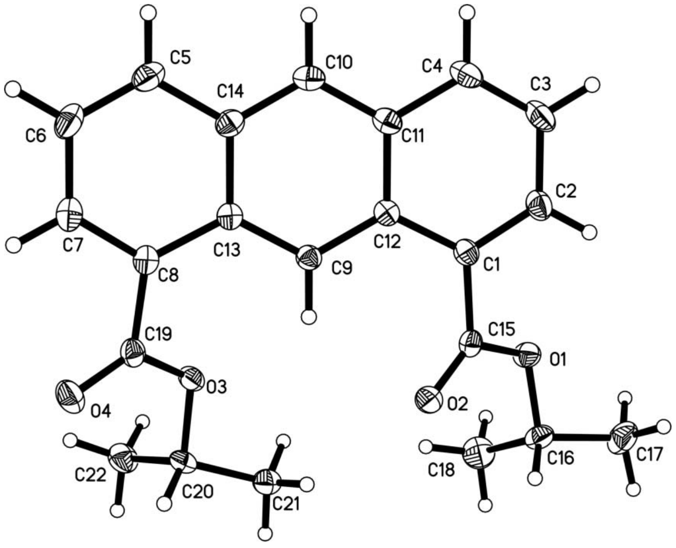

Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

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