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Di-*n*-propyl naphthalene-1,4-dicarboxylate

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Key indicators

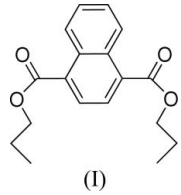
Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.001 Å
R factor = 0.034
wR factor = 0.101
Data-to-parameter ratio = 17.3

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

In the title compound, $C_{18}H_{20}O_4$, the two ester groups are twisted away from the attached ring by 38.36 (3)° and 36.00 (3)°. The crystal structure is stabilized by π–π stacking interactions.

Comment

Naphthalene-1,4-dicarboxylic 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). Previously, we have reported the crystal structures of dimethyl naphthalene-1,4-dicarboxylate (Jing *et al.*, 2005), diphenyl naphthalene-1,4-dicarboxylate (Jing, Qin, Gu *et al.*, 2006) and diethyl naphthalene-1,4-dicarboxylate (Jing, Qin, Zhang *et al.*, 2006). We now report the crystal structure of the title compound, (I).



(I)

The bond lengths and angles in (I) are normal. The naphthalene ring system is slightly distorted from planarity, with a dihedral angle of 5.40 (4)° between the two rings. As a result of steric effects, the 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/C15/C16 planes form dihedral angles of 38.36 (3) and 36.00 (3)°, respectively, with the plane formed by atoms C1–C4/C9/C10. Two intramolecular C—H···O hydrogen bonds are observed in the molecular structure (Table 1).

The crystal structure is stabilized by π–π stacking interaction between the C1–C4/C9/C10 rings at (x, y, z) and ($1-x$, $1-y$, $1-z$), whose centroids are separated by 3.4778 (5) Å.

Experimental

Naphthalene-1,4-dicarboxylic acid (2 mmol) and an excess of thionyl chloride (6 mmol) in dioxane (20 ml) was boiled under reflux for 6 h. The solution was distilled at reduced pressure. An excess of *n*-propanol (6 mmol) was added to the resulting yellow solid and heated under reflux for one day. After the solution had cooled to ambient temperature, water (25 ml) was added, affording a colourless solid. The solution was filtered to remove the propanol and water. The filter cake was dissolved in methanol and left to stand for one month at ambient temperature, after which colourless single crystals suitable for X-ray diffraction were obtained.

Crystal data

$C_{18}H_{20}O_4$
M_r = 300.34
Monoclinic, $P2_1/c$
a = 13.1091 (2) Å
b = 7.2172 (1) Å
c = 16.9995 (4) Å
β = 108.719 (1)°
V = 1523.27 (5) Å^3
Z = 4
D_x = 1.310 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 (2) K
Block, colourless
0.37 × 0.33 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: none
14297 measured reflections
3487 independent reflections
3179 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.101
S = 1.00
3487 reflections
202 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 0.3354P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0085 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O3	0.95	2.36	2.9731 (13)	122
C8—H8···O1	0.95	2.41	2.9974 (14)	120

H atoms were placed in calculated positions, with C—H = 0.95–0.99 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). The methyl groups were allowed to rotate but not to tip.

Data collection: *RAPID-AUTO* (Rigaku/MSC, 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* (Bruker, 1997); software used to prepare material for publication: *SHELXTL97*.

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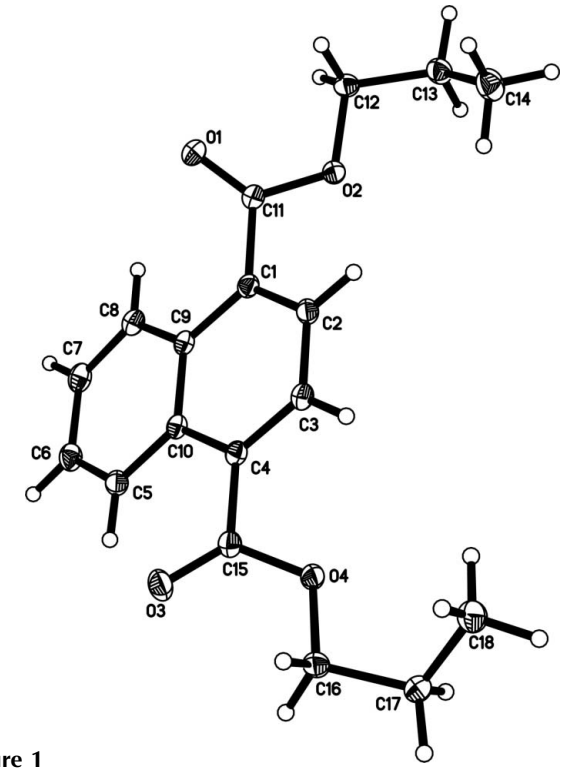

Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

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