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Isopropyl 3,5-dinitrobenzoate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.056
wR factor = 0.155
Data-to-parameter ratio = 15.6

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

In the title compound, $C_{10}H_{10}N_2O_6$, the dinitrobenzoate moiety is nearly planar. In the crystal structure, the molecules are stacked along the b axis, without any π–π interaction.

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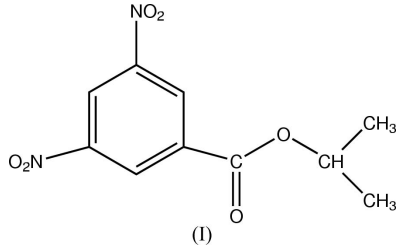
Comment

Dinitrobenzoate compounds are of interest because of their biological activities. Some synthetic dinitrobenzoate compounds have shown useful properties in DNA and oligosaccharide synthesis (Olive, 1979; Huang *et al.*, 2004). Dinitrobenzoic acid derivatives are effective radiation sensitizers in tumour treatment (Kagitani *et al.*, 1984). Furthermore, a series of 3,5-dinitrobenzoic acid esters has also been synthesized and their anti-creatinine effects have been studied (Yu & Yang, 2002). These properties prompted us to find new methods to synthesize these compounds and to study their structures and activities. We report here the crystal structure of the title compound, (I).



(I)

The bond lengths and angles in (I) show normal values (Table 1). Except for atoms C9 and C10, the other non-H atoms of the molecule lie in a plane with an r.m.s deviation of 0.065 Å. In the crystal structure, the molecules are stacked along the b axis, without any π–π interaction (Fig. 2). An N2···O5($\frac{1}{2}-x$, $y-\frac{1}{2}$, $\frac{1}{2}-z$) short contact of 2.937 (4) Å is observed.

Experimental

Compound (I) was synthesized according to the literature procedure of Bartlett & Trachtenberg (1958). A crystal suitable for X-ray analysis was grown from a solution in methanol at room temperature by slow evaporation.

Crystal data

$C_{10}H_{10}N_2O_6$
M_r = 254.20
Monoclinic, $P2_1/n$
a = 9.886 (2) Å
b = 5.7887 (11) Å
c = 20.646 (4) Å
β = 96.129 (4)°
V = 1174.8 (4) Å^3
Z = 4
D_x = 1.437 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 670 reflections
θ = 2.2–19.9°
μ = 0.12 mm^{-1}
T = 293 (2) K
Prism, colourless
0.40 × 0.20 × 0.04 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.953, T_{max} = 0.995
6612 measured reflections
2567 independent reflections
1209 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 27.0°
$h = -12 \rightarrow 12$
$k = -7 \rightarrow 6$
$l = -26 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.155
S = 0.97
2567 reflections
165 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C7	1.499 (4)	C8—O6	1.473 (3)
C3—N1	1.476 (3)	N1—O1	1.221 (3)
C5—N2	1.468 (3)	N1—O2	1.223 (3)
C7—O5	1.203 (3)	N2—O3	1.214 (3)
C7—O6	1.324 (3)	N2—O4	1.220 (3)
C6—C1—C7	117.5 (2)	O2—N1—C3	117.7 (3)
C2—C1—C7	122.9 (3)	O3—N2—O4	124.1 (3)
O5—C7—O6	125.6 (3)	O4—N2—C5	117.5 (3)
O5—C7—C1	122.0 (3)	C7—O6—C8	117.0 (2)
O1—N1—O2	124.1 (2)		
C2—C1—C7—O6	5.0 (4)	C6—C5—N2—O4	−4.0 (4)
C2—C3—N1—O1	5.5 (4)	O5—C7—O6—C8	−2.0 (4)
C4—C3—N1—O2	6.9 (3)	C1—C7—O6—C8	177.8 (2)
C4—C5—N2—O3	−4.0 (4)		

All H atoms were included in the riding-model approximation, with C—H distances of 0.93 (aromatic H atoms), 0.96 (methyl H atoms) and 0.98 Å (tertiary H atom). The isotropic displacement parameters were set equal to $1.2U_{eq}$ of the carrier atom for the aromatic and tertiary H atoms, and to $1.5U_{eq}$ of the carrier atom for methyl H atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Bruker, 2001); software used to prepare material for publication: *SHELXTL-NT*.

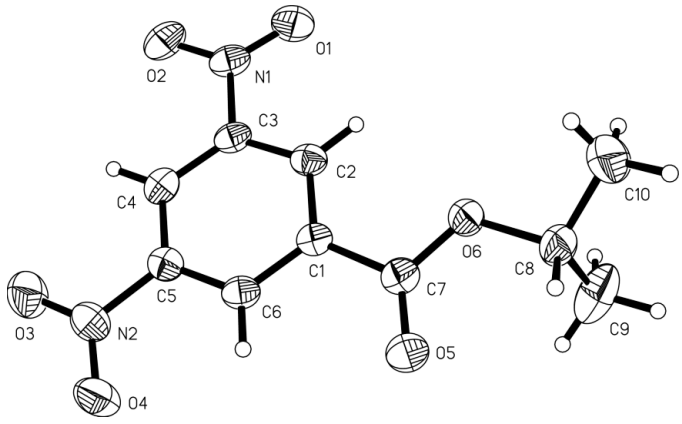


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level.

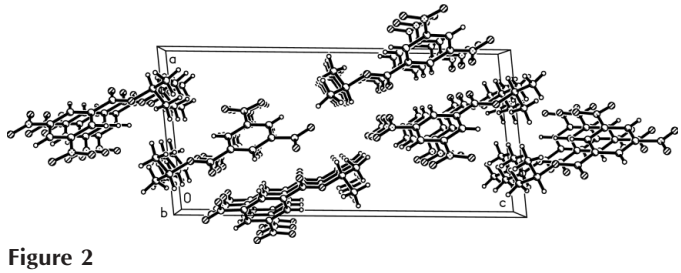


Figure 2
The packing of (I), viewed along the *b* axis.

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