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Propyl 3,6-diphenyl-1,4-dihydro-1,2,4,5-tetrazine-1-carboxylate

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Key indicators

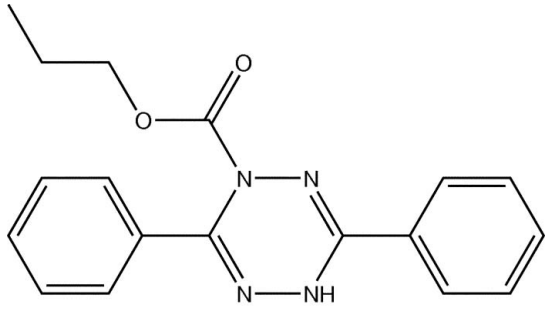
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.036
wR factor = 0.105
Data-to-parameter ratio = 7.2

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

The title compound, $C_{18}H_{18}N_4O_2$, was prepared from propyl chloroformate and 3,6-diphenyl-1,2-dihydro-1,2,4,5-tetrazine. The central six-membered ring has a boat conformation. In the crystal structure, molecules are linked *via* N—H···N [N···N = 3.015 (4) Å] and C—H···O [C···O = 3.265 (6) Å] hydrogen bonds to form extended chains along [100].

Comment

1,2,4,5-Tetrazine derivatives have a high potential for biological activity, possessing a wide range of antiviral and antitumour properties, and these derivatives have been widely used in pesticides and herbicides (Sauer, 1996). In a continuation of our work on the structure–activity relationships of 1,2,4,5-tetrazine derivatives (Hu *et al.*, 2002, 2004), we have obtained a yellow crystalline compound as the product of the reaction of propyl chloroformate and 3,6-diphenyl-1,2-dihydro-1,2,4,5-tetrazine. The structure of our product, (I), was solved using single-crystal X-ray diffraction.



(I)

The molecular structure of (I) is illustrated in Fig. 1. In (I), atoms N2, C3, N5 and C6 are coplanar [deviations within 0.0348 (16) Å] and atoms N1 and N4 deviate from the plane by 0.456 (5) and 0.380 (5) Å, respectively, indicating a boat conformation. In the crystal structure, molecules are linked *via* N—H···N [N···N = 3.015 (4) Å] and C—H···O [C···O = 3.265 (6) Å] hydrogen bonds to form extended chains along [100] (see Table 1 for hydrogen-bond geometries).

Experimental

The title compound was prepared according to the procedure of Rao & Hu, (2004). A solution of the compound in ethanol was concentrated gradually at room temperature to afford yellow prisms (m.p. 414–415 K).

Crystal data

$C_{18}H_{18}N_4O_2$
M_r = 322.36
Orthorhombic, $Pna2_1$
a = 10.212 (3) Å
b = 10.051 (2) Å
c = 16.611 (3) Å
V = 1705.0 (7) Å^3
Z = 4
D_x = 1.256 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10.7–12.5°
μ = 0.09 mm^{-1}
T = 298 (2) K
Prism, yellow
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.967, T_{max} = 0.983
1699 measured reflections
1584 independent reflections
997 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.2°
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 12$
$l = -19 \rightarrow 1$
3 standard reflections
frequency: 60 min
intensity decay: 0.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.106
S = 1.05
1584 reflections
219 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0614P)^2 + 0.0145P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.012 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H3···N2^{i}	0.86	2.32	3.015 (4)	139
C14—H14···O1^{i}	0.93	2.34	3.265 (6)	172

Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{5}{2}, z$.

H atoms were included in calculated positions [C—H(methyl) = 0.96, other C—H =0.97, N—H = 0.86 Å] and refined using a riding model, with U_{iso}(H) equal to 1.2 (or 1.5 for methyl H atoms) times U_{eq}(parent atom). In the absence of significant anomalous dispersion effects, Friedel pairs were merged.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Version 1.05; Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

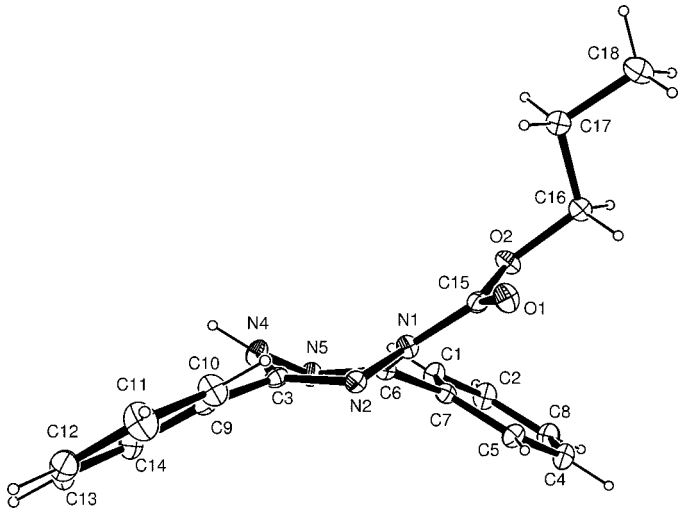


Figure 1
The structure of (I), shown with 30% probability displacement ellipsoids.

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