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3,6-Dipropyl-*N*,*N*′-di-*o*-tolyl-1,2,4,5-tetrazine-1,4-dicarboxamide

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.067
wR factor = 0.261
Data-to-parameter ratio = 13.7

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

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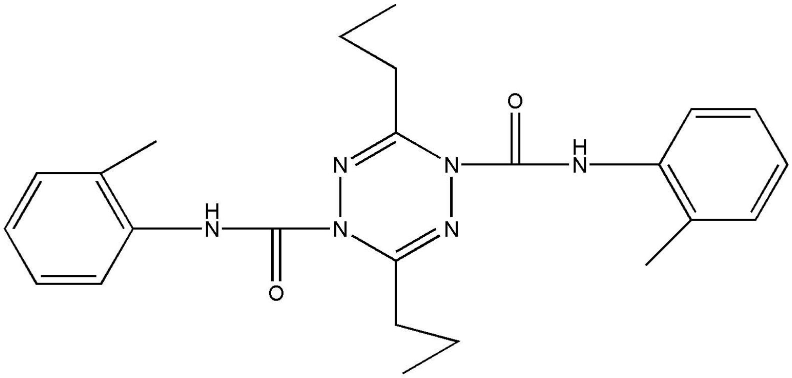
The title compound, $C_{24}H_{30}N_6O_2$, crystallizes with two molecules in the asymmetric unit, both lying on twofold rotation axes. In both molecules, the central tetrazine ring adopts a boat conformation.

Comment

s-Tetrazine derivatives have a high potential for biological activity, possessing a wide range of antiviral and antitumour properties (Neunhoeffer, 1984). These derivatives have been widely used as pesticides and herbicides (Sauer, 1996). In continuation of our research on structure–activity relationships of *s*-tetrazine derivatives (Hu *et al.*, 2002, 2004), we have obtained a colourless crystalline compound, (I). The structural identity of (I) was confirmed using single-crystal X-ray diffraction.



(I)

The molecular structure of (I) is illustrated in Fig. 1. Selected bond lengths and angles are listed in Table 1. Compound (I) crystallizes in the monoclinic space group *C*2/*c* with two symmetry-independent molecules having slightly different geometries (Table 1), both lying on twofold rotation axes. In both molecules, the central tetrazine ring adopts a boat conformation; atoms N2 (molecule 1) and N5 (molecule 2) and their symmetry equivalents deviate from the mean planes formed by the other four atoms of the tetrazine rings by 0.488 (8) and 0.470 (8) Å, respectively.

Experimental

The title compound was obtained by refluxing 2-methylphenyl isocyanate (0.04 mol) with 3,6-dipropyl-1,6-dihydro-1,2,4,5-tetrazine (0.01 mol) in chloroform (60 ml) for 72 h and subsequent removal of the solvent. A solution of the compound in butanone was concen-

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trated gradually at room temperature to afford colourless crystals (m.p. 399–401 K).

Crystal data

$C_{24}H_{30}N_6O_2$
$M_r = 434.54$
Monoclinic, $C2/c$
$a = 24.083$ (3) Å
$b = 7.784$ (3) Å
$c = 24.461$ (4) Å
$\beta = 90.70$ (3)°
$V = 4585$ (2) Å^3
$Z = 8$

$D_x = 1.259$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 9.7$–10.9°
$\mu = 0.08$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.30 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.965$, $T_{max} = 0.984$
4874 measured reflections
4117 independent reflections
2511 reflections with $I > 2\sigma(I)$

$R_{int} = 0.058$
$\theta_{max} = 25.2$°
$h = 0 \rightarrow 28$
$k = -1 \rightarrow 9$
$l = -29 \rightarrow 29$
3 standard reflections every 100 reflections intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.261$
$S = 1.19$
4117 reflections
301 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0885P)^2 + 14.4993P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N2—C9^i	1.391 (6)	N5—C29^i	1.402 (6)
N2—N3	1.426 (5)	N5—N6	1.426 (5)
N3—C9	1.273 (6)	N6—C29	1.279 (6)
C9^i—N2—N3	115.3 (4)	C29—N6—N5	113.6 (4)
C9—N3—N2	112.8 (4)	N3—C9—N2^i	119.1 (4)
C29^i—N5—N6	115.6 (4)	N6—C29—N5^i	119.2 (4)
C9^i—N2—N3—C9	41.4 (5)	N2—N3—C9—N2^i	−3.9 (6)
C29^i—N5—N6—C29	−39.7 (5)	N5—N6—C29—N5^i	4.2 (6)

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

H atoms were placed in calculated positions and refined using a riding model. They were given isotropic displacement parameters equal to 1.2 (or 1.5 for methyl H atoms) times the equivalent isotropic displacement parameters of their parent atoms, and C—H distances were set at 0.93 Å for the aromatic H atoms and 0.96 Å for those of the methyl groups.

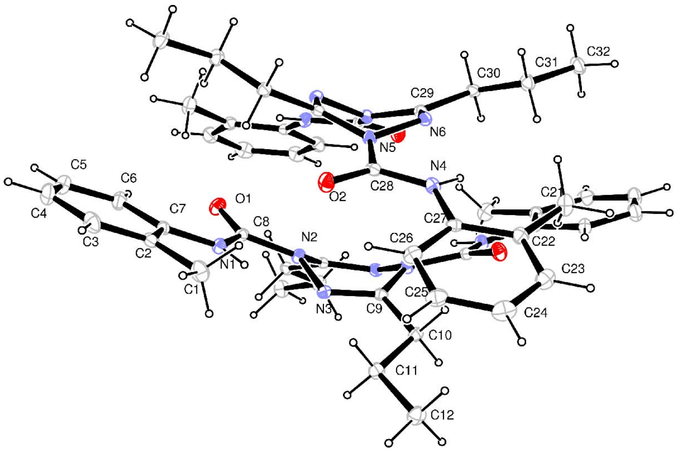

Figure 1
The two independent molecules of (I), shown with 30% probability displacement ellipsoids. Unlabelled atoms are related to labelled atoms by the symmetry operator $(-x, y, \frac{1}{2} - z)$

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (McArdle, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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