

1,3-Dibenzylthymine

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Key indicators

Single-crystal X-ray study

T = 273 K

Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$

R factor = 0.039

wR factor = 0.098

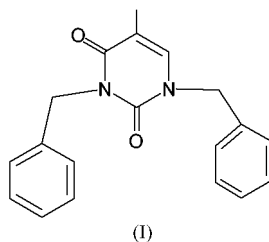
Data-to-parameter ratio = 16.7

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

In the title compound, $\text{C}_{19}\text{H}_{18}\text{N}_2\text{O}_2$, the two phenyl rings are located on the same side of the thymine ring, resembling the two front claws of a crab. The crystal structure involves some weak $\text{C}-\text{H}\cdots\text{O}$ interactions.

Comment

Nucleobases are important in biology, being responsible for a wide range of biochemical processes, such as complementary base pairing in genetic information storage and transfer, molecular recognition and some enzymatic reactions (Bazzicalupi *et al.*, 2001). As a result, considerable efforts have been made to investigate thymine and its derivatives. These studies include the crystal structure and theoretical investigation of the electronic properties of *cis*-5-hydroperoxy-6-hydroxy-5,6-dihydrothymine (Jolibois *et al.*, 1998); the low-frequency vibrational spectrum of 1-methylthymine (Kirin *et al.*, 1975); the synthesis, cation reporter properties and recognition of 1-methylthymine by a macrocyclic zinc(II) complex (Koike *et al.*, 1998).



In an earlier study, we reported the synthesis and crystal structure of 1-benzylthymine (Ding *et al.*, 2002). Since then, a new thymine derivative, 1,3-dibenzylthymine, (I), has been obtained and its crystal structure is reported here.

The title compound contains two phenyl rings and one heterocyclic ring (Fig. 1). The two phenyl rings, (C1–C6) and (C14–C19) are each essentially planar, with average deviations from planarity of 0.007 and 0.008 Å , respectively. The atoms of the thymine ring (C8, C9, C11, C12, N1, N2) are coplanar, with an average deviation of 0.013 Å ; the value in 1-benzylthymine is very similar, *viz.* 0.010 Å .

The two phenyl rings are located on the same side of the thymine ring, resembling the two front claws of a crab. The dihedral angles between the mean planes of the thymine ring and the phenyl rings are 81.7 (2) $^\circ$ (phenyl ring C1–C6) and 67.4 (2) $^\circ$ (phenyl ring C14–C19).

Moreover, the non-bonded interactions are also different in 1,3-dibenzylthymine and in 1-benzylthymine. In the former, there are only weak $\text{C}-\text{H}\cdots\text{O}$ interactions C7–

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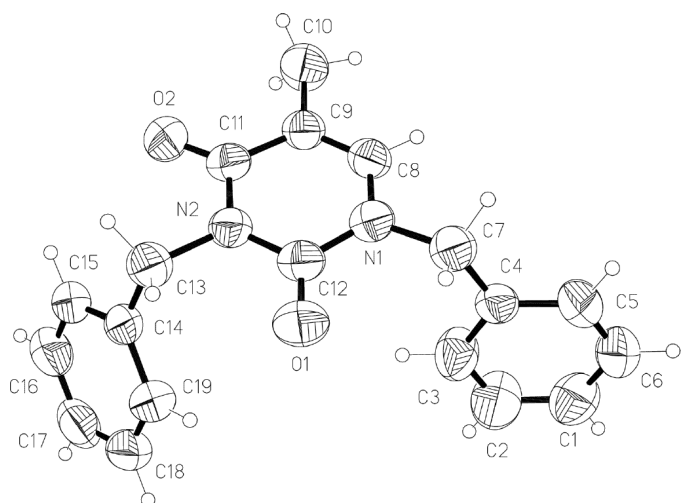


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

$H7B \cdots O1(x - \frac{1}{2}, \frac{5}{2} - y, -z)$ and $C18-H18 \cdots O2(1 + x, y, z)$ with $C \cdots O$ distances of 3.391 (2) and 3.481 (2) Å, respectively; the angles at $H7B$ and $H18$ are 151 and 169°, respectively. On the other hand, in 1-benzylthymine, there are strong $N-H \cdots O$ hydrogen bond interactions with $N \cdots O$ distances of 2.872 (5) Å and 2.834 (5) Å and significant $\pi \cdots \pi$ interactions between neighboring phenyl rings separated by 3.46 Å.

Experimental

The title compound was synthesized through the benzylation of 0.25 g thymine with 0.54 ml benzyl bromide by neutralization of 2.00 g potassium carbonate, and catalysis of 0.10 g tetrabutylammonium bromide in the mixed solvents *N,N'*-dimethylacetamide and diethylene glycol ($v/v = 1:10$); the reaction time was five minutes in a National NN-S568WFS 900 W microwave oven. Single crystals suitable for X-ray data collection were obtained by recrystallization from a mixture of ethanol and dichloromethane.

Crystal data

$C_{19}H_{18}N_2O_2$
 $M_r = 306.35$
 Orthorhombic, $P2_12_12_1$
 $a = 8.7466$ (10) Å
 $b = 8.8637$ (10) Å
 $c = 20.720$ (3) Å
 $V = 1606.3$ (3) Å³
 $Z = 4$
 $D_x = 1.267$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 599 reflections
 $\theta = 2.3$ – 18.0°
 $\mu = 0.08$ mm⁻¹
 $T = 273$ (2) K
 Block, colorless
 $0.45 \times 0.28 \times 0.25$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: none
 7934 measured reflections
 3508 independent reflections

2618 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.026$
 $\theta_{max} = 27.0^\circ$
 $h = -10 \rightarrow 11$
 $k = -11 \rightarrow 7$
 $l = -20 \rightarrow 26$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.098$
 $S = 0.97$
 3508 reflections
 210 parameters
 H-atoms parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.12$ e Å⁻³
 $\Delta\rho_{min} = -0.12$ e Å⁻³
 Extinction correction: *SHELXL*
 Extinction coefficient: 0.16 (SU?)

Table 1

Selected geometric parameters (Å, °).

O1—C12	1.2168 (18)	C4—C7	1.507 (2)
O2—C11	1.2206 (19)	C5—C6	1.381 (3)
N1—C12	1.373 (2)	C8—C9	1.327 (2)
N1—C8	1.376 (2)	C9—C11	1.441 (2)
N1—C7	1.470 (2)	C9—C10	1.503 (2)
N2—C12	1.385 (2)	C13—C14	1.510 (3)
N2—C11	1.4047 (19)	C14—C19	1.377 (2)
N2—C13	1.4819 (19)	C14—C15	1.377 (3)
C1—C6	1.356 (3)	C15—C16	1.375 (3)
C1—C2	1.361 (3)	C16—C17	1.366 (3)
C2—C3	1.377 (3)	C17—C18	1.368 (3)
C3—C4	1.367 (2)	C18—C19	1.380 (3)
C4—C5	1.371 (2)		
N1—C7—C4	114.68 (13)	N2—C13—C14	112.84 (13)

In the absence of significant anomalous dispersion effects, the 1480 Friedel pairs were merged and the absolute configuration can not be determined from the crystallographic experiment.

All H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93 Å for Csp^2-H , 0.96 Å for $C(\text{methyl})-H$ and 0.97 Å for $C(\text{methylene})-H$. Isotropic displacement parameters were set to $1.5U_{eq}$ (methylene and methyl) and $1.2U_{eq}$ (other H atoms) of the carrier atom.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINTE* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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