Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,3-Bis(4-methylbenzyl)pyrimidine-2,4(1*H*,3*H*)-dione

Gong-Chun Li, Xiao-Ping Song, Li-Ke Zhang, Jiao-Jiao Cui and Feng-Ling Yang*

College of Chemistry and Chemical Engineering, Xuchang University, Xuchang, Henan Province 461000, People's Republic of China
Correspondence e-mail: actaeli@gmail.com

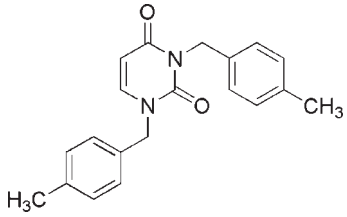
Received 1 December 2009; accepted 12 December 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.088; wR factor = 0.161; data-to-parameter ratio = 13.7.

In the title molecule, $C_{20}H_{20}N_2O_2$, the central pyrimidine ring forms dihedral angles of 71.9 (1) and 69.8 (1)° with the two benzene rings. In the crystal, weak intermolecular C—H···O hydrogen bonds link molecules into centrosymmetric dimers. The crystal packing exhibits also π–π interactions as indicated by short distances of 3.674 (2) Å between the centroids of the pyrimidine rings of neighbouring molecules.

Related literature

For the crystal structure of 1,3-bis(4-chlorobenzyl)pyrimidine-2,4(1*H*,3*H*)-dione, see: Yang & Li (2006).



Experimental

Crystal data

$C_{20}H_{20}N_2O_2$
M_r = 320.38
Triclinic, $P\overline{1}$
a = 9.4182 (19) Å
b = 10.102 (2) Å
c = 10.448 (2) Å
α = 66.25 (3)°
β = 80.79 (3)°
γ = 71.18 (3)°
V = 860.7 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2006)
T_{min} = 0.984, T_{max} = 0.984
8622 measured reflections
3001 independent reflections
2529 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.088
$wR(F^2)$ = 0.161
S = 1.27
3001 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O2^{i}	0.93	2.50	3.430 (4)	174

Symmetry code: (i) $-x, -y+1, -z+2$.

Data collection: *CrystalClear* (Rigaku/MSC, 2006); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Natural Science Foundation of Henan Province, China (grant No. 082300420110) and the Natural Science Foundation of Henan Province Education Department, China (grant No. 2007150036).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2673).

References

Rigaku/MSC (2006). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yang, F.-L. & Li, G.-C. (2006). *Acta Cryst.* E**62**, o3405–o3406.

supplementary materials

Acta Cryst. (2010). E**66**, o193 [**doi:10.1107/S1600536809053586**]

1,3-Bis(4-methylbenzyl)pyrimidine-2,4(1*H*,3*H*)-dione

G.-C. Li, X.-P. Song, L.-K. Zhang, J.-J. Cui and F.-L. Yang

Comment

In continuation of our search for new biologically active pyrimidine derivatives (Yang & Li, 2006), we present here the title compound (I).

In (I) (Fig. 1), all bond lengths and angles are normal and correspond to those observed in the related 1,3-bis(4-chlorobenzyl)pyrimidine-2,4(1*H*,3*H*)-dione (Yang & Li, 2006). The central pyrimidine ring forms dihedral angles of 71.9 (1)° and 69.8 (1)° with the two benzene rings, respectively. Weak intermolecular C—H···O hydrogen bonds (Table 1) link molecules into centrosymmetric dimers. The crystal packing exhibits also π-π interactions proved by short distances of 3.674 (2) Å between the centroids of pyrimidine rings from the neighbouring molecules.

Experimental

Uracil (0.56 g, 5 mmol) and anhydrous potassium carbonate (0.84 g, 6 mmol) were mixed in *N*,*N*-dimethylformamide (20 ml). A solution of 4-methyl-benzyl chloride (0.70 g, 5 mmol) in acetone (10 ml) was then added dropwise, with stirring, at room temperature, and the mixture was stirred for another 10 h and then refluxed for 4 h. The solvent was evaporated *in vacuo* and the residue was washed with water. The resulting white precipitate was filtered off and purified by column chromatography on silica gel (petroleum ether:ethyl acetate = 2:1). The title compound was recrystallized from ethanol and single crystals of (I) were obtained by slow evaporation.

Refinement

All H atoms were placed in calculated positions, with C—H = 0.93 - 0.97 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2–1.5 U_{eq}(C).

Figures

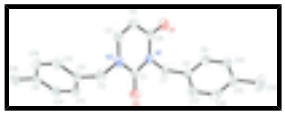


Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms omitted for clarity.

1,3-Bis(4-methylbenzyl)pyrimidine-2,4(1*H*,3*H*)-dione

Crystal data

$C_{20}H_{20}N_2O_2$	$Z = 2$
$M_r = 320.38$	$F(000) = 340$
Triclinic, $P\overline{1}$	$D_x = 1.236$ Mg m^{-3}

a = 9.4182 (19) Å	Mo $K\alpha$ radiation, λ = 0.71073 Å
b = 10.102 (2) Å	Cell parameters from 2459 reflections
c = 10.448 (2) Å	θ = 2.1–27.9°
α = 66.25 (3)°	μ = 0.08 mm^{-1}
β = 80.79 (3)°	T = 293 K
γ = 71.18 (3)°	Prism, colourless
V = 860.7 (3) $Å^3$	0.20 × 0.20 × 0.20 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer	3001 independent reflections
Radiation source: fine-focus sealed tube	2529 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.034
Detector resolution: 28.5714 pixels mm^{-1}	θ_{max} = 25.0°, θ_{min} = 2.1°
phi and ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2006)	$k = -11 \rightarrow 12$
T_{min} = 0.984, T_{max} = 0.984	$l = -12 \rightarrow 12$
8622 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.088	H-atom parameters constrained
$wR(F^2)$ = 0.161	$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.3734P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.27	$(\Delta/\sigma)_{max} < 0.001$
3001 reflections	$\Delta\rho_{max}$ = 0.14 e $Å^{-3}$
219 parameters	$\Delta\rho_{min}$ = −0.17 e $Å^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. Software + citation

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4982 (3)	0.1871 (3)	0.6026 (3)	0.0711 (7)
O2	0.3392 (2)	0.4909 (3)	0.8542 (2)	0.0661 (7)
N1	0.4156 (2)	0.3369 (3)	0.7299 (2)	0.0452 (6)
N2	0.2678 (3)	0.5867 (3)	0.6284 (3)	0.0491 (6)
C1	0.3407 (3)	0.4728 (3)	0.7458 (3)	0.0483 (7)
C2	0.6580 (3)	0.1972 (3)	0.8500 (3)	0.0431 (7)
C3	0.1828 (3)	0.7346 (3)	0.6372 (4)	0.0596 (9)
H3A	0.1960	0.8147	0.5494	0.072*
H3B	0.2227	0.7467	0.7105	0.072*
C4	0.3402 (3)	0.4340 (4)	0.4937 (3)	0.0562 (8)
H4	0.3370	0.4235	0.4099	0.067*
C5	0.2677 (3)	0.5635 (4)	0.5079 (3)	0.0543 (8)
H5	0.2143	0.6422	0.4330	0.065*
C6	0.7652 (3)	0.0843 (3)	0.8165 (3)	0.0529 (8)
H6	0.7358	0.0149	0.7973	0.064*
C7	0.4931 (3)	0.2105 (3)	0.8525 (3)	0.0521 (8)
H7A	0.4827	0.1170	0.8550	0.063*
H7B	0.4451	0.2249	0.9372	0.063*
C8	−0.2911 (3)	0.7765 (3)	0.7206 (3)	0.0492 (8)
C9	0.4242 (3)	0.3092 (4)	0.6070 (3)	0.0526 (8)
C10	−0.0848 (4)	0.8346 (4)	0.5629 (3)	0.0577 (8)
H10	−0.0510	0.8844	0.4730	0.069*
C11	0.0171 (3)	0.7490 (3)	0.6673 (3)	0.0473 (7)
C12	0.9150 (4)	0.0739 (4)	0.8113 (3)	0.0614 (9)
H12	0.9854	−0.0040	0.7901	0.074*
C13	−0.0374 (4)	0.6768 (4)	0.7999 (3)	0.0599 (9)
H13	0.0286	0.6189	0.8726	0.072*
C14	−0.1891 (4)	0.6899 (3)	0.8254 (3)	0.0582 (9)
H14	−0.2231	0.6392	0.9150	0.070*
C15	0.9639 (4)	0.1749 (4)	0.8365 (3)	0.0630 (10)
C16	−0.4572 (3)	0.7930 (4)	0.7502 (4)	0.0696 (10)
H16A	−0.5029	0.8770	0.7787	0.104*
H16B	−0.4712	0.7025	0.8235	0.104*
H16C	−0.5030	0.8099	0.6671	0.104*
C17	0.7049 (4)	0.2967 (4)	0.8803 (3)	0.0601 (9)
H17	0.6349	0.3714	0.9064	0.072*
C18	−0.2361 (4)	0.8480 (4)	0.5894 (4)	0.0610 (9)
H18	−0.3022	0.9066	0.5168	0.073*
C19	0.8569 (4)	0.2856 (4)	0.8720 (4)	0.0717 (11)
H19	0.8869	0.3548	0.8909	0.086*
C20	1.1291 (4)	0.1673 (6)	0.8239 (4)	0.1041 (16)
H20A	1.1884	0.0636	0.8601	0.156*
H20B	1.1462	0.2195	0.8764	0.156*
H20C	1.1572	0.2137	0.7274	0.156*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0713 (16)	0.0577 (15)	0.0837 (18)	−0.0011 (12)	−0.0192 (13)	−0.0334 (13)
O2	0.0646 (15)	0.0773 (16)	0.0552 (14)	−0.0105 (12)	−0.0044 (11)	−0.0303 (13)
N1	0.0379 (13)	0.0480 (15)	0.0434 (14)	−0.0112 (11)	−0.0041 (11)	−0.0106 (12)
N2	0.0424 (14)	0.0438 (14)	0.0534 (16)	−0.0082 (11)	−0.0015 (12)	−0.0138 (12)
C1	0.0381 (17)	0.0513 (19)	0.052 (2)	−0.0148 (14)	0.0023 (14)	−0.0162 (16)
C2	0.0462 (17)	0.0411 (16)	0.0355 (15)	−0.0103 (14)	−0.0092 (13)	−0.0066 (13)
C3	0.0519 (19)	0.0480 (19)	0.076 (2)	−0.0136 (16)	0.0004 (16)	−0.0216 (17)
C4	0.053 (2)	0.057 (2)	0.058 (2)	−0.0112 (17)	−0.0080 (16)	−0.0218 (17)
C5	0.0481 (19)	0.058 (2)	0.0452 (19)	−0.0149 (16)	−0.0077 (14)	−0.0052 (16)
C6	0.055 (2)	0.0476 (18)	0.0524 (19)	−0.0145 (15)	−0.0082 (15)	−0.0126 (15)
C7	0.0487 (18)	0.0488 (18)	0.0469 (18)	−0.0157 (15)	−0.0059 (14)	−0.0032 (14)
C8	0.0509 (19)	0.0464 (18)	0.0543 (19)	−0.0124 (15)	0.0041 (15)	−0.0262 (15)
C9	0.0415 (18)	0.054 (2)	0.062 (2)	−0.0143 (16)	−0.0056 (15)	−0.0203 (17)
C10	0.059 (2)	0.056 (2)	0.0474 (19)	−0.0160 (16)	0.0000 (15)	−0.0094 (16)
C11	0.0463 (17)	0.0376 (16)	0.0568 (19)	−0.0090 (14)	−0.0008 (15)	−0.0192 (14)
C12	0.052 (2)	0.060 (2)	0.054 (2)	−0.0038 (17)	−0.0051 (16)	−0.0103 (17)
C13	0.056 (2)	0.060 (2)	0.0489 (19)	−0.0025 (16)	−0.0081 (16)	−0.0143 (16)
C14	0.060 (2)	0.054 (2)	0.0499 (19)	−0.0094 (17)	0.0092 (16)	−0.0181 (16)
C15	0.050 (2)	0.073 (2)	0.047 (2)	−0.0214 (19)	−0.0100 (15)	0.0015 (17)
C16	0.053 (2)	0.081 (3)	0.083 (3)	−0.0202 (18)	0.0078 (18)	−0.042 (2)
C17	0.058 (2)	0.056 (2)	0.068 (2)	−0.0105 (17)	−0.0118 (17)	−0.0254 (17)
C18	0.051 (2)	0.070 (2)	0.057 (2)	−0.0112 (17)	−0.0121 (16)	−0.0191 (18)
C19	0.075 (3)	0.072 (2)	0.079 (3)	−0.034 (2)	−0.024 (2)	−0.021 (2)
C20	0.055 (2)	0.149 (4)	0.084 (3)	−0.042 (3)	−0.010 (2)	−0.007 (3)

Geometric parameters (Å, °)

O1—C9	1.221 (4)	C8—C14	1.382 (4)
O2—C1	1.215 (3)	C8—C16	1.513 (4)
N1—C1	1.390 (4)	C10—C18	1.381 (4)
N1—C9	1.405 (4)	C10—C11	1.378 (4)
N1—C7	1.478 (3)	C10—H10	0.9300
N2—C5	1.370 (4)	C11—C13	1.383 (4)
N2—C1	1.386 (4)	C12—C15	1.371 (5)
N2—C3	1.482 (4)	C12—H12	0.9300
C2—C17	1.376 (4)	C13—C14	1.383 (4)
C2—C6	1.381 (4)	C13—H13	0.9300
C2—C7	1.512 (4)	C14—H14	0.9300
C3—C11	1.512 (4)	C15—C19	1.375 (5)
C3—H3A	0.9700	C15—C20	1.520 (4)
C3—H3B	0.9700	C16—H16A	0.9600
C4—C5	1.322 (4)	C16—H16B	0.9600
C4—C9	1.439 (4)	C16—H16C	0.9600
C4—H4	0.9300	C17—C19	1.391 (4)
C5—H5	0.9300	C17—H17	0.9300

C6—C12	1.375 (4)	C18—H18	0.9300
C6—H6	0.9300	C19—H19	0.9300
C7—H7A	0.9700	C20—H20A	0.9600
C7—H7B	0.9700	C20—H20B	0.9600
C8—C18	1.374 (4)	C20—H20C	0.9600
C1—N1—C9	125.6 (3)	C18—C10—C11	121.3 (3)
C1—N1—C7	117.3 (3)	C18—C10—H10	119.4
C9—N1—C7	117.1 (3)	C11—C10—H10	119.4
C5—N2—C1	121.7 (3)	C10—C11—C13	117.7 (3)
C5—N2—C3	119.8 (3)	C10—C11—C3	120.8 (3)
C1—N2—C3	118.5 (3)	C13—C11—C3	121.5 (3)
O2—C1—N2	122.4 (3)	C6—C12—C15	122.0 (3)
O2—C1—N1	122.7 (3)	C6—C12—H12	119.0
N2—C1—N1	114.9 (3)	C15—C12—H12	119.0
C17—C2—C6	118.5 (3)	C14—C13—C11	120.7 (3)
C17—C2—C7	121.2 (3)	C14—C13—H13	119.6
C6—C2—C7	120.3 (3)	C11—C13—H13	119.6
N2—C3—C11	111.9 (2)	C8—C14—C13	121.5 (3)
N2—C3—H3A	109.2	C8—C14—H14	119.3
C11—C3—H3A	109.2	C13—C14—H14	119.3
N2—C3—H3B	109.2	C12—C15—C19	117.3 (3)
C11—C3—H3B	109.2	C12—C15—C20	121.7 (4)
H3A—C3—H3B	107.9	C19—C15—C20	120.9 (4)
C5—C4—C9	120.5 (3)	C8—C16—H16A	109.5
C5—C4—H4	119.8	C8—C16—H16B	109.5
C9—C4—H4	119.8	H16A—C16—H16B	109.5
C4—C5—N2	122.8 (3)	C8—C16—H16C	109.5
C4—C5—H5	118.6	H16A—C16—H16C	109.5
N2—C5—H5	118.6	H16B—C16—H16C	109.5
C12—C6—C2	120.5 (3)	C2—C17—C19	120.1 (3)
C12—C6—H6	119.8	C2—C17—H17	120.0
C2—C6—H6	119.8	C19—C17—H17	120.0
N1—C7—C2	112.6 (2)	C10—C18—C8	121.4 (3)
N1—C7—H7A	109.1	C10—C18—H18	119.3
C2—C7—H7A	109.1	C8—C18—H18	119.3
N1—C7—H7B	109.1	C15—C19—C17	121.6 (3)
C2—C7—H7B	109.1	C15—C19—H19	119.2
H7A—C7—H7B	107.8	C17—C19—H19	119.2
C18—C8—C14	117.5 (3)	C15—C20—H20A	109.5
C18—C8—C16	121.4 (3)	C15—C20—H20B	109.5
C14—C8—C16	121.1 (3)	H20A—C20—H20B	109.5
O1—C9—N1	120.2 (3)	C15—C20—H20C	109.5
O1—C9—C4	125.3 (3)	H20A—C20—H20C	109.5
N1—C9—C4	114.4 (3)	H20B—C20—H20C	109.5
C5—N2—C1—O2	−178.4 (3)	C5—C4—C9—O1	−177.7 (3)
C3—N2—C1—O2	−1.2 (4)	C5—C4—C9—N1	2.5 (4)
C5—N2—C1—N1	1.6 (4)	C18—C10—C11—C13	−0.1 (5)
C3—N2—C1—N1	178.9 (2)	C18—C10—C11—C3	179.8 (3)

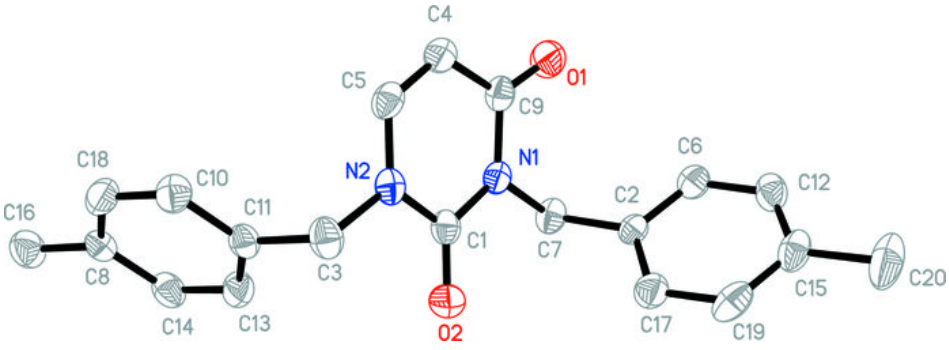
C9—N1—C1—O2	−178.8 (3)	N2—C3—C11—C10	−103.7 (3)
C7—N1—C1—O2	1.1 (4)	N2—C3—C11—C13	76.1 (4)
C9—N1—C1—N2	1.2 (4)	C2—C6—C12—C15	−1.1 (5)
C7—N1—C1—N2	−178.9 (2)	C10—C11—C13—C14	0.5 (5)
C5—N2—C3—C11	80.2 (3)	C3—C11—C13—C14	−179.3 (3)
C1—N2—C3—C11	−97.2 (3)	C18—C8—C14—C13	0.8 (5)
C9—C4—C5—N2	0.0 (5)	C16—C8—C14—C13	−178.6 (3)
C1—N2—C5—C4	−2.2 (4)	C11—C13—C14—C8	−0.9 (5)
C3—N2—C5—C4	−179.5 (3)	C6—C12—C15—C19	2.1 (5)
C17—C2—C6—C12	−1.1 (4)	C6—C12—C15—C20	−177.1 (3)
C7—C2—C6—C12	178.7 (3)	C6—C2—C17—C19	2.3 (5)
C1—N1—C7—C2	−95.8 (3)	C7—C2—C17—C19	−177.5 (3)
C9—N1—C7—C2	84.1 (3)	C11—C10—C18—C8	0.0 (5)
C17—C2—C7—N1	74.8 (4)	C14—C8—C18—C10	−0.3 (5)
C6—C2—C7—N1	−105.0 (3)	C16—C8—C18—C10	179.0 (3)
C1—N1—C9—O1	177.0 (3)	C12—C15—C19—C17	−0.9 (5)
C7—N1—C9—O1	−2.8 (4)	C20—C15—C19—C17	178.3 (3)
C1—N1—C9—C4	−3.2 (4)	C2—C17—C19—C15	−1.3 (5)
C7—N1—C9—C4	176.9 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O2^{i}	0.93	2.50	3.430 (4)	174

Symmetry codes: (i) −*x*, −*y*+1, −*z*+2.

Fig. 1


C4
C5
O1
C9
C18
C10
N2
N1
C6
C12
C16
C11
C2
C8
C3
C1
C7
C15
C20
C14
C13
O2
C17
C19