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

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.104
Data-to-parameter ratio = 16.0

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

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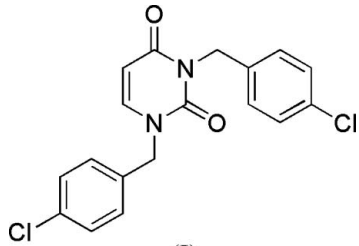
In the crystal structure of the title compound, $C_{18}H_{14}Cl_2N_2O_2$, there are weak intermolecular C—H···O hydrogen-bond interactions. In the title molecule, the plane of the pyrimidine ring makes angles of 71.6 (1) and 71.72 (9)° with the planes of the two benzene rings.

Comment

Pyrimidine derivatives are very important molecules in biology and have many applications as pesticides and pharmaceutical agents (Condon *et al.*, 1993). For example, imazosulfuron, ethirmol and mepanipyrim have been commercialized as agrochemicals (Maeno *et al.*, 1990). Pyrimidine derivatives have also been developed as antiviral agents, such as AZT (azidothymidine), which is the most widely used anti-AIDS drug (Gilchrist, 1997).



(I)

In the quest for further biologically active pyrimidine compounds, the title compound, (I), has been synthesized and its crystal structure determined (Fig. 1). In (I), the pyrimidine ring (C8–C11/N1/N2) is almost planar, with a maximum deviation of 0.033 (2) Å for C8. The dihedral angles formed by the C1–C6 and C13–C18 benzene rings with the pyrimidine ring are 71.6 (1) and 71.72 (9)°, respectively. The dihedral angle between the two benzene rings is 82.0 (1)°. In the crystal structure, there are weak intermolecular C—H···O hydrogen-bond interactions (Table 1).

Experimental

Uracil (5 mmol) and anhydrous potassium carbonate (6 mmol) were mixed in dimethylformamide (20 ml). A solution of 4-chlorobenzyl chloride (0.81 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 were obtained.

Crystal data

$C_{18}H_{14}Cl_2N_2O_2$
M_r = 361.21
Monoclinic, $C2/c$
a = 28.118 (9) Å
b = 8.941 (3) Å
c = 14.291 (5) Å
β = 108.047 (5)°
V = 3416.0 (19) Å^3
Z = 8
D_x = 1.405 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 294 (2) K
Block, colourless
0.30 × 0.26 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.891, T_{max} = 0.926
9294 measured reflections
3476 independent reflections
2133 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.104
S = 1.00
3476 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0406P)^2 + 1.7213P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O2	0.97	2.36	2.725 (3)	101
C12—H12A···O2	0.97	2.39	2.736 (3)	100
C12—H12A···O2^{i}	0.97	2.49	3.388 (3)	154
C17—H17···O1^{ii}	0.93	2.38	3.267 (3)	160

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, y+1, -z+\frac{1}{2}$.

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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References

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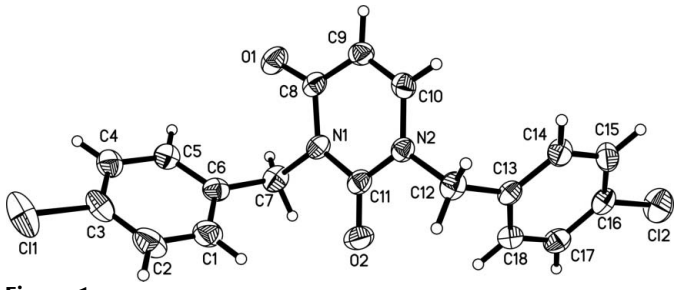

Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

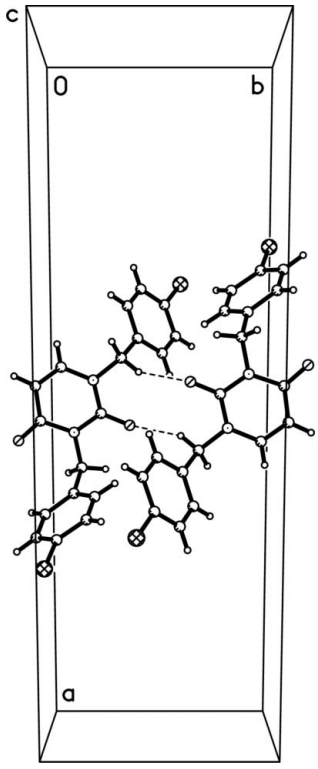

Figure 2
A view of the intermolecular C12—H12A···O2 hydrogen-bond interactions (dashed lines) in (I).

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