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1,3-Bis(2-furylmethylidene)-3,4,5,6-tetrahydropyrimidin-2(1*H*)-one

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.063
wR factor = 0.169
Data-to-parameter ratio = 12.6

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

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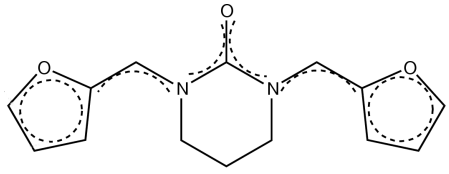
The title compound, $C_{14}H_{14}N_2O_3$, possesses C_s symmetry, with the central CH_2 and C=O atoms of the tetrahydropyrimidin-2-one group lying on the mirror plane. The molecule is bow-shaped, with two symmetry-related intramolecular C—H···O hydrogen bonds. In the crystal structure, the molecules stack along the *a* axis and there are no short intermolecular contacts.

Comment

Furan derivatives have been of great interest for many years. These compounds play an important role in the development of chemistry related to sterilization and enzymatic reactions. In order to investigate the crystal structure of furan derivatives, we report here the structure of a new compound, (I) (Fig. 1). The molecule has C_s symmetry, atoms C8, C6 and O2 lying on a mirror plane. The bond lengths and angles are in the normal ranges. The molecule is bow-shaped, with two symmetry-related intramolecular C5—H5···O2 hydrogen bonds (see Table 1 for details). The dihedral angle between the two furan rings is 16.2 (4)°. The torsion angles C1—C5—N1—C6, C1—C5—N1—C7 and C5—N1—C7—C8 are −174.6 (3), 2.9 (3) and 161.5 (3)°, respectively. Atom C8 deviates from the plane defined by atoms N1, N1^{i}, C7^{i} and C7 by 0.628 (3) Å [symmetry code: (i) $x, \frac{1}{2}-y, z$]. As a result of the conjugation through the double bonds, C5=N1 and C6=O2, the furan ring and atoms C5, N1, C6 and O2 are essentially coplanar [mean deviation from the overall plane is 0.043 (4) Å]. The dihedral angle between the furan ring and the plane defined by atoms N1, N1^{i}, C7^{i} and C7 is 13.6 (4)°.



(I)

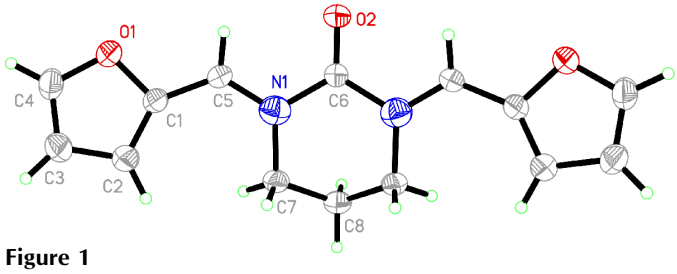


Figure 1
The structure of the title compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

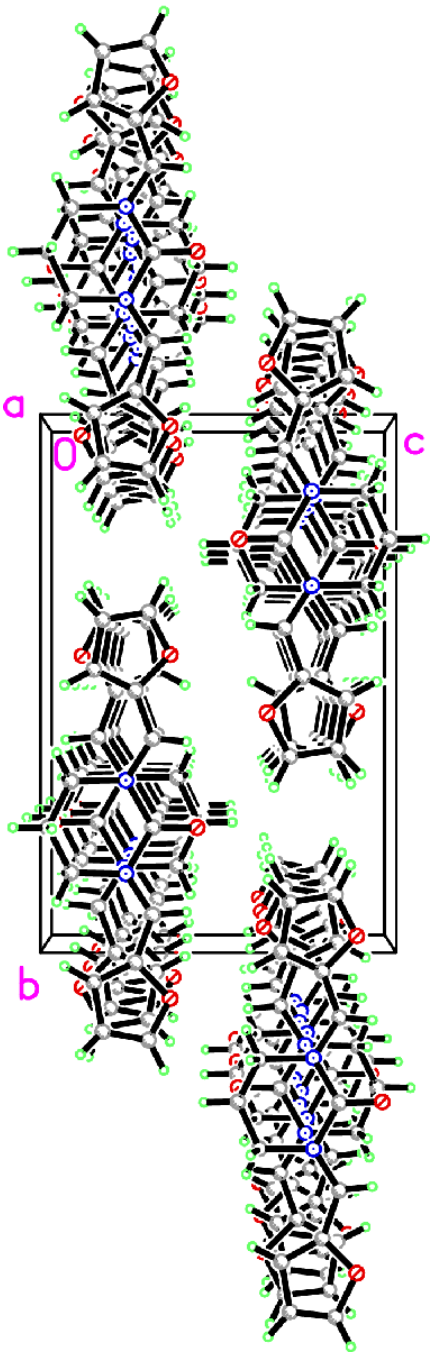


Figure 2
The crystal packing of the title compound, (I), viewed along the *a* axis.

In the crystal structure, the molecules stack along the *a* axis with no short molecular contacts (<3.2 Å) (see Fig. 2).

Experimental

Furaldehyde and 1,3-diaminopropane are available commercially (Aldrich) and were used without further purification. Furaldehyde (0.2 mmol, 19.2 mg) and 1,3-diaminopropane (0.1 mmol, 7.4 mg) were dissolved in MeOH (5 ml). The mixture was stirred for 10 min and then transferred to a stainless steel bomb, which was sealed, heated at 423 K for 12 h, and cooled gradually to room temperature. Yellow block-shaped crystals of the title compound were collected, washed three times with methanol and dried in a vacuum desiccator containing anhydrous $CaCl_2$ (yield 71.2%). Analysis found: C 64.9, H 5.5, N 10.9%; calculated for $C_{14}H_{14}N_2O_3$: C 65.1, H 5.5, N 10.8%.

Crystal data

$C_{14}H_{14}N_2O_3$
M_r = 258.27
Orthorhombic, *Pnma*
a = 7.725 (5) Å
b = 15.670 (9) Å
c = 10.342 (6) Å
V = 1251.9 (13) Å^3
Z = 4
D_x = 1.370 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 812 reflections
θ = 2.3–18.4°
μ = 0.10 mm^{-1}
T = 298 (2) K
Block, yellow
0.37 × 0.33 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.965, T_{max} = 0.990
5987 measured reflections
1151 independent reflections
619 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
θ_{max} = 25.0°
$h = -9 \rightarrow 9$
$k = -18 \rightarrow 14$
$l = -12 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.170
S = 0.91
1151 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0945P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O2	0.93	2.38	2.755 (4)	104

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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