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(*RS*)-2-[(Furan-2-carbonyl)amino]propionic acid

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Key indicators

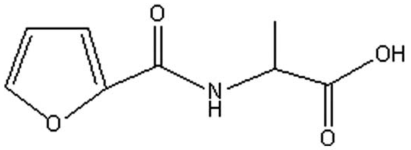
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.132
Data-to-parameter ratio = 12.4

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

In the asymmetric unit of the title compound, $C_8H_9NO_4$, there is a pair of independent molecules in different conformations. Each of these conformers forms a dimer *via* a pair of N—H···O hydrogen bonds with the respective enantiomer. The enantiomers within each dimer are related by inversion. The dimers are connected by strong O—H···O hydrogen bonds. In addition, there are C—H···O hydrogen bonds, as well as π–π interactions, between the furan rings of each dimer. Bond lengths and angles are unexceptional.

Comment

Furan derivatives are well known in many marine organisms (Faulkner, 2001). Some show important bioactivities, such as antitumor (Phuwapraisirsan *et al.*, 2004) and diabetes treatment activity (Hwang *et al.*, 2002). This is the reason why they have attracted our interest. This study follows our previous study on (*S*)-methyl 2-[(furan-2-carbonyl)amino]-3-phenylpropanoate (Zeng *et al.*, 2006).



(I)

There are two independent molecules in the asymmetric unit of the title compound, (I), with different conformations. The conformers differ in the orientation of the 2-carbonyl O atoms with regard to the furan O atoms (Fig. 1). Each of these conformers is linked to its respective enantiomer by a pair of N—H···O hydrogen bonds (Table 1), forming a dimer (Fig. 2). Each dimer is centrosymmetric and it is situated on a space-group inversion centre. The graph-set motif within each dimer is $R_2^2(10)$ (Bernstein *et al.*, 1995). Both dimers are interconnected by strong O—H···O hydrogen bonds. There are also C—H···O hydrogen bonds in (I) (Table 1).

In addition, there are π–π interactions between the furan rings of each dimer. The distance between the centroids of the ring O1/C1–C4 and of its enantiomer (symmetry code: $1 - x$, $1 - y$, $1 - z$) is 3.8167 (15) Å, and between the centroids of the ring O5/C9–C12 and of its enantiomer (symmetry code: $2 - x$, $2 - y$, $-z$) is 3.7516 (13) Å.

Experimental

DL-Methyl 2-aminopropionate hydrochloride (0.70 g, 5 mmol) was added to dichloromethane (6 ml), followed by the addition of triethylamine (1.5 ml). After stirring for 15 min, the precipitate was filtered off. Furan-2-carbonyl chloride (0.5 ml, 5 mmol) in dichloromethane (3 ml) was added dropwise to the filtrate at 288–293 K. The mixture reacted at room temperature for 2 h; it was then filtered and the solid was collected and dissolved in 12 ml of 10% aqueous NaOH (10 ml) with ethanol (2 ml). The mixture was stirred at room temperature for 24 h, then acidified with 10% HCl to pH = 2, and extracted four times with 10 ml of ethyl acetate. The organic phase was dried by anhydrous sodium sulfate overnight and the solvent was removed by distillation under reduced pressure. The pale-yellow solid residue was dissolved in ethanol at room temperature. Colourless triclinic crystals suitable for X-ray analysis (m.p. 442 K, in 83.0 wt% yield) grew over several days when the solution was exposed to air. Elemental analysis calculated for $C_8H_9NO_4$: C 52.46, H 4.95, N 7.65%; found: C 52.38, H 4.98, N 7.70%.

Crystal data

$C_8H_9NO_4$
$M_r = 183.16$
Triclinic, $P\bar{1}$
$a = 8.4240\ (11)$ Å
$b = 10.1388\ (13)$ Å
$c = 10.8220\ (14)$ Å
$\alpha = 104.146\ (2)^\circ$
$\beta = 94.137\ (2)^\circ$
$\gamma = 106.413\ (2)^\circ$
$V = 849.78\ (19)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.12$ mm^{-1}
$T = 173\ (2)$ K
$0.48 \times 0.46 \times 0.16$ mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.946$, $T_{\max} = 0.982$
6167 measured reflections
2954 independent reflections
2547 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.132$
$S = 1.08$
2954 reflections
239 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.45$ e Å^{-3}
$\Delta\rho_{\min} = -0.36$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O8—H8···O2	0.84	1.75	2.581 (2)	171
N2—H2···O7$^{\rm i}$	0.88	2.17	3.000 (2)	157
O4—H4···O6$^{\rm ii}$	0.84	1.74	2.572 (2)	173
N1—H1···O3$^{\rm iii}$	0.88	2.13	2.941 (2)	153
N2—H2···O5	0.88	2.35	2.704 (2)	104
C11—H11···O4$^{\rm iv}$	0.95	2.55	3.312 (3)	138
C14—H14···O8$^{\rm v}$	1.00	2.59	3.454 (2)	144

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $x, y-1, z$; (iii) $-x+1, -y, -z+1$; (iv) $x, y+1, z$; (v) $-x+1, -y+1, -z$.

All the H atoms were seen in the difference Fourier map. Nevertheless, the H atoms were placed in idealized positions [C—H = 1.00 Å for CH (methine), 0.98 Å for CH_3 (methyl), 0.95 Å for CH (aryl), N—H = 0.88 Å and O—H = 0.84 Å] and refined using a riding model, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(carrier atom) or $1.5U_{\rm eq}$(methyl C).

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

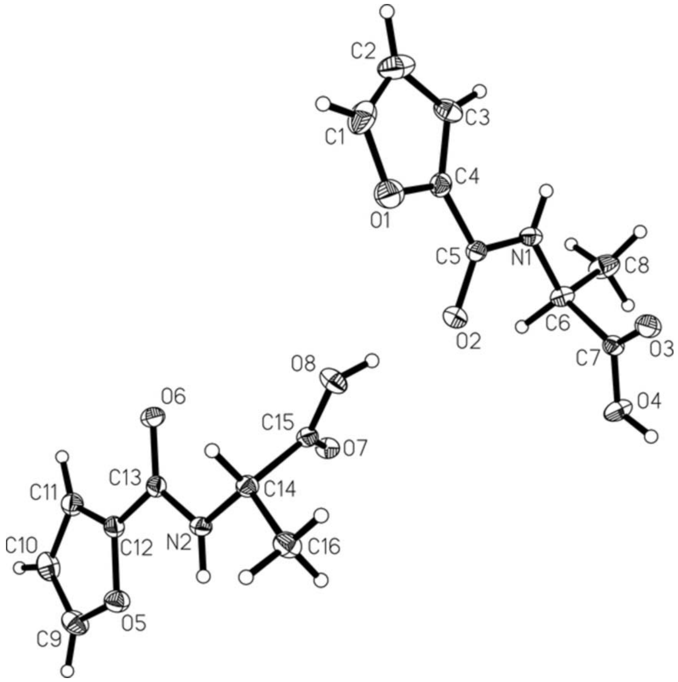


Figure 1
The asymmetric unit of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

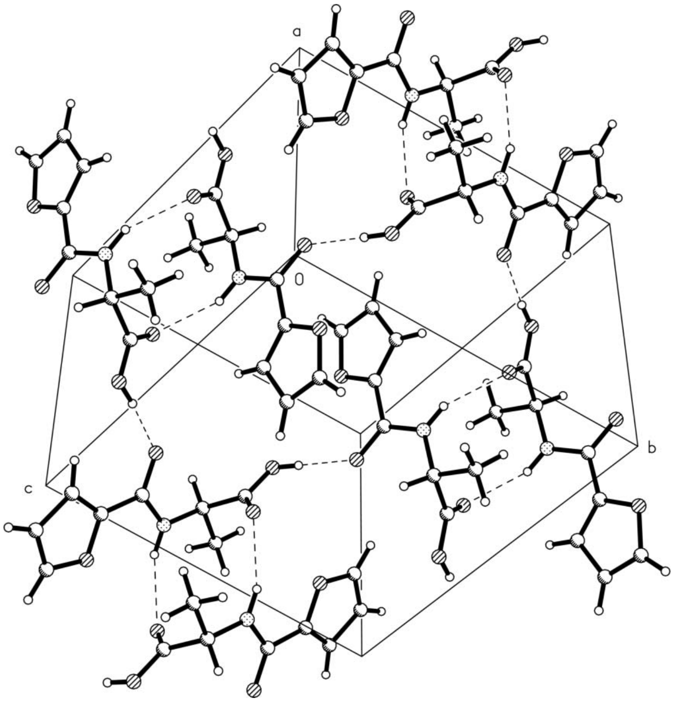


Figure 2
The crystal packing of the title compound, showing the O—H···O and N—H···O hydrogen bonds (dashed lines).

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