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Methyl 3-(1*H*-pyrrol-2-ylcarboxamido)propionate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.128
Data-to-parameter ratio = 17.1

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

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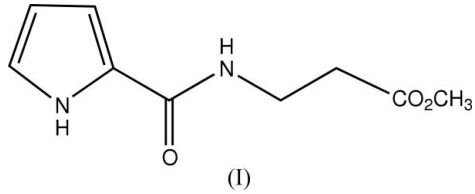
In the crystal structure of the title compound, $C_9H_{12}N_2O_3$, intermolecular N—H···O hydrogen bonds link the molecules into two-dimensional sheets.

Comment

Pyrrole derivatives are well known in many marine organisms (Faulkner, 2001) and some of them are bioactive substances (Tasdemir *et al.*, 2002).



(I)

In our search for bioactive compounds, a series of pyrrol-2-ylcarbonylamino acid esters, including the title compound, (I), have been synthesized by reaction of amino acid esters with 2-(trichloroacetyl)pyrrole or 1-methyl-2-(trichloroacetyl)-pyrrole. Pharmacological studies have shown that (I) moderately inhibits *Streptococcus faecalis* and *Micrococcus luteus*. We report here the crystal structure of (I).

Bond lengths and angles are unexceptional and are in good agreement with the corresponding values in 3-(pyrrol-2-ylcarboxamido)propanoic acid (Zeng *et al.*, 2005).

There are two kinds of intermolecular hydrogen bonds (Table 1) in the crystal structure. N2—H···O1^{ii} hydrogen bonds link molecules into one-dimensional chains (Fig. 2), while individual chains are linked by N1—H···O2^{i} hydrogen bonds, generating two-dimensional sheets (also shown in Fig. 2)

Experimental

The hydrochloric acid salt of methyl 3-aminopropionate (0.70 g, 5 mmol) and 2-trichloroacetylpyrrole (1.06 g, 5 mmol) were added to acetonitrile (12 ml), followed by the dropwise addition of triethylamine (1.4 ml). The mixture was stirred at room temperature for 12 h and then poured into water. After filtration, the precipitate was collected as a pale-brown solid. The impure product was dissolved in methanol at room temperature. Colorless plate-shaped crystals suitable for X-ray analysis (m.p. 407 K, yield 94.9%) grew over a period of 10 d when the solution was exposed to air. ^{1}H NMR ($CDCl_3$, 500 Hz): 10.40 (*brs*, 1H), 6.93–6.91 (*m*, 1H), 6.76 (*brs*, 1H), 6.62–6.60 (*m*, 1H), 6.21–6.20 (*m*, 1H), 3.70 (*s*, 3H), 3.71–3.67 (*m*, 2H), 2.64 (*t*, 2H); IR (KBr): 3364, 3326, 3115, 1725, 1625, 1565, 1531, 1345, 1191, 1109. Analysis calculated for $C_9H_{12}N_2O_3$: C 55.09, H 6.16, N 14.28%; found: C 55.03, H 6.32, N 14.50%.

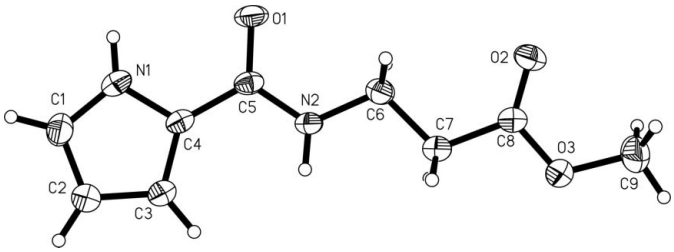


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Crystal data

$C_9H_{12}N_2O_3$
M_r = 196.21
Orthorhombic, *Pbca*
a = 10.1525 (14) Å
b = 13.1586 (18) Å
c = 14.922 (2) Å
V = 1993.5 (5) Å^3
Z = 8
D_x = 1.307 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2641 reflections
θ = 2.7–23.4°
μ = 0.10 mm^{-1}
T = 293 (2) K
Plate, colorless
0.45 × 0.41 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.957, T_{max} = 0.990
12061 measured reflections
2194 independent reflections
1263 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 27.2°
$h = -13 \rightarrow 12$
$k = -16 \rightarrow 16$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.128
S = 1.00
2194 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.7536P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.020
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.12	2.893 (2)	149
N2—H2···O1^{ii}	0.86	2.11	2.954 (2)	167

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

H atoms were positioned geometrically (C—H = 0.97 Å for CH_2, 0.96 Å for CH_3, C—H = 0.93 Å for aromatic CH and N—H = 0.86 Å) and refined using a riding model, with $U_{iso} = 1.2U_{eq}$ ($1.5U_{eq}$ for the methyl group) of the parent atom.

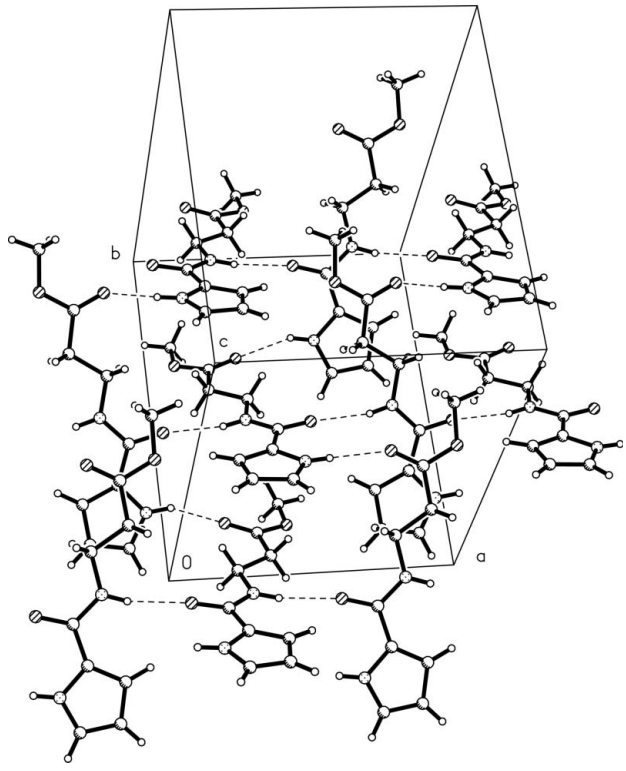


Figure 2
The crystal packing of (I), showing the two-dimensional sheet formed by hydrogen bonds (dashed lines).

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

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References

Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Faulkner, D. J. (2001). *Nat. Prod. Rep.* **18**, 1–49.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Tasdemir, D., Mallon, R., Greenstein. M., Feldberg, L. R., Kim, S. C., Collins, K., Wojciechowicz, D., Mangalindan, G. C., Concepcion, G. P., Harper, M. K. & Ireland, C. M. (2002). *J. Med. Chem.* **45**, 529–532.
Zeng, X. C., Xu, S. H., Gu, J. & Liu, P. R. (2005). *Chin. J. Struct. Chem.* **24**, 779–782.