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# Ethyl 4-methyl-1*H*-pyrrole-3-carboxylate

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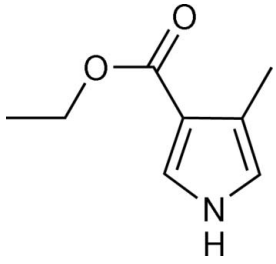
Key indicators: single-crystal X-ray study; $T$ = 200 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.045; $wR$ factor = 0.124; data-to-parameter ratio = 18.0.

The molecule of the title compound, $C_8H_{11}NO_2$, is nearly planar, possibly due to aromatic conjugation of the carboxylate group with the aromatic pyrrole ring. The molecules form infinite supramolecular chains along the [101] direction *via* intermolecular N—H···O hydrogen bonding.

## Related literature

The title compound was prepared according to a synthesis described by Büchel *et al.* (1994). For the structure of a related compound, see: Baures *et al.* (2002). For related literature, see: Cheng *et al.* (1976).



## Experimental

*Crystal data*

$C_8H_{11}NO_2$
$M_r$ = 153.18
Monoclinic, $C2/c$
$a$ = 11.3757 (5) Å
$b$ = 10.9074 (4) Å
$c$ = 14.1470 (4) Å
$\beta$ = 110.644 (2)°
$V$ = 1642.64 (11) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 200 (2) K
0.23 × 0.12 × 0.08 mm

*Data collection*

Nonius KappaCCD diffractometer
Absorption correction: none
3569 measured reflections
1859 independent reflections
1468 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.124
$S$ = 1.06
1859 reflections
103 parameters
Only H-atom displacement parameters refined
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H101···O2$^{i}$ | 0.88 | 1.96 | 2.809 (2) | 163 |

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

Data collection: *COLLECT* (Nonius, 2004); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK* program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank Anna Zangl for experimental support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2348).

## References

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# supplementary materials

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# Ethyl 4-methyl-1*H*-pyrrole-3-carboxylate

**T. Kerscher, P. Klüfers, W. Kügel and C. Müller**

## Comment

The title compound, $C_8H_{11}NO_2$, was prepared as a tentative ligand for transition metal complexes.

The molecular structure is shown in Fig. 1. The molecule is nearly planar which might be due to aromatic conjugation of the carboxyl group with the aromatic pyrrol ring, and packing effects for the ethyl group (Fig. 2).

In the crystal structure, the molecules are connected to form supramolecular chains *via* N—H···O hydrogen bonds (Table 1).

For the structures of a series of imidazole-4,5-dicarboxylic-acid derivatives see Baures *et al.* (2002).

## Experimental

The title compound was prepared according to a synthesis described in Büchel *et al.* (1994). The title compound was obtained upon reaction of 4-methylphenylsulfonylmethylisocyanide with 2-butenoic acid ethyl ester in a mixture of dry ether and dimethylsulfoxide (2:1) under reductive conditions (NaH) at room temperature. After 30 minutes the excess sodium hydride was quenched by the addition of water. After another 30 minutes the reaction mixture was extracted with diethylether three times. The combined organic phases were combined yielding a yellow oil. After column chromatography on aluminium oxide with dichloromethane as solvent and removal of the solvent of the first fraction, light yellow crystals were obtained.

## Refinement

All H atoms were placed in calculated positions with C—H = 0.95 (aromatic), 0.98(methyl), 0.99 Å (methylene) an N—H = 0.88 Å, and refined as riding on their parent atoms with one common isotropic displacement parameter.

## Figures

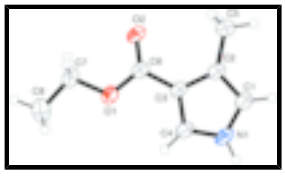

Fig. 1. The molecular structure of (I), with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

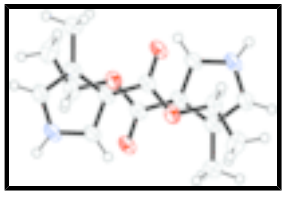

Fig. 2. Packing of two closest non-hydrogen-bonded neighbours of (I) in a normal view.

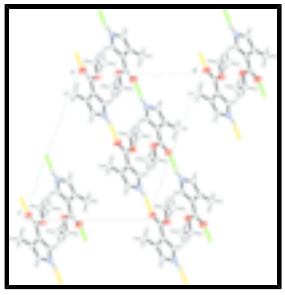

Fig. 3. Hydrogen-bonded chains, view along [0 − 1 0], 0.0 < *y* < 0.5 only.

**Ethyl 4-methyl-1*H*-pyrrole-3-carboxylate**

*Crystal data*

| | |
|---|---|
| $C_8H_{11}NO_2$ | $F_{000}$ = 656 |
| $M_r$ = 153.18 | $D_x$ = 1.239 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 8547 reflections |
| *a* = 11.3757 (5) Å | θ = 3.1–27.5º |
| *b* = 10.9074 (4) Å | μ = 0.09 mm$^{-1}$ |
| *c* = 14.1470 (4) Å | *T* = 200 (2) K |
| β = 110.644 (2)º | Block, light yellow |
| *V* = 1642.64 (11) Å$^3$ | 0.23 × 0.12 × 0.08 mm |
| *Z* = 8 | |

*Data collection*

| | |
|---|---|
| Enraf–Nonius KappaCCD diffractometer | 1468 reflections with $I > 2\sigma(I)$ |
| Radiation source: rotating anode | $R_{int}$ = 0.020 |
| Monochromator: MONTEL, graded multilayered X-ray optics | $\theta_{max}$ = 27.5º |
| *T* = 200(2) K | $\theta_{min}$ = 3.4º |
| ω scan | *h* = −14→14 |
| Absorption correction: none | *k* = −14→14 |
| 3569 measured reflections | *l* = −17→17 |
| 1859 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.045 | Only H-atom displacement parameters refined |
| $wR(F^2)$ = 0.124 | $w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 1.2343P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 1.06 | $(\Delta/\sigma)_{max} < 0.001$ |

| | |
|---|---|
| 1859 reflections | $\Delta\rho_{max} = 0.21$ e Å$^{-3}$ |
| 103 parameters | $\Delta\rho_{min} = -0.19$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.17019 (10) | 0.42295 (10) | 0.01285 (8) | 0.0377 (3) |
| O2 | 0.02995 (10) | 0.26964 (12) | −0.03239 (8) | 0.0436 (3) |
| C3 | 0.18984 (13) | 0.26544 (14) | 0.12870 (10) | 0.0307 (3) |
| N1 | 0.33745 (12) | 0.23332 (12) | 0.27728 (9) | 0.0376 (3) |
| H101 | 0.4069 | 0.2405 | 0.3302 | 0.0626 (18)* |
| C2 | 0.15334 (14) | 0.16238 (14) | 0.17421 (11) | 0.0332 (3) |
| C6 | 0.12186 (13) | 0.31647 (14) | 0.02949 (11) | 0.0316 (3) |
| C4 | 0.30409 (14) | 0.30630 (15) | 0.19499 (11) | 0.0350 (4) |
| H41 | 0.3509 | 0.3738 | 0.1845 | 0.0626 (18)* |
| C7 | 0.10894 (16) | 0.47856 (16) | −0.08579 (12) | 0.0399 (4) |
| H71 | 0.0194 | 0.4948 | −0.0970 | 0.0626 (18)* |
| H72 | 0.1136 | 0.4230 | −0.1397 | 0.0626 (18)* |
| C5 | 0.03638 (16) | 0.08732 (17) | 0.13147 (13) | 0.0460 (4) |
| H51 | 0.0417 | 0.0157 | 0.1746 | 0.0626 (18)* |
| H52 | 0.0274 | 0.0600 | 0.0633 | 0.0626 (18)* |
| H53 | −0.0366 | 0.1371 | 0.1285 | 0.0626 (18)* |
| C1 | 0.24662 (15) | 0.14637 (15) | 0.26568 (11) | 0.0371 (4) |
| H11 | 0.2483 | 0.0848 | 0.3136 | 0.0626 (18)* |
| C8 | 0.1760 (2) | 0.59605 (18) | −0.08746 (16) | 0.0552 (5) |
| H81 | 0.1696 | 0.6507 | −0.0345 | 0.0626 (18)* |
| H82 | 0.1377 | 0.6355 | −0.1535 | 0.0626 (18)* |
| H83 | 0.2647 | 0.5789 | −0.0755 | 0.0626 (18)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0391 (6) | 0.0381 (6) | 0.0306 (6) | 0.0009 (5) | 0.0055 (5) | 0.0037 (4) |
| O2 | 0.0361 (6) | 0.0550 (7) | 0.0280 (6) | −0.0057 (5) | −0.0031 (4) | 0.0044 (5) |
| C3 | 0.0289 (7) | 0.0349 (8) | 0.0246 (7) | 0.0040 (6) | 0.0049 (6) | −0.0026 (6) |
| N1 | 0.0339 (7) | 0.0438 (8) | 0.0257 (6) | 0.0035 (6) | −0.0013 (5) | −0.0025 (5) |
| C2 | 0.0315 (7) | 0.0366 (8) | 0.0274 (7) | 0.0023 (6) | 0.0055 (6) | −0.0025 (6) |
| C6 | 0.0288 (7) | 0.0367 (8) | 0.0274 (7) | 0.0039 (6) | 0.0076 (6) | −0.0016 (6) |
| C4 | 0.0335 (8) | 0.0359 (8) | 0.0292 (7) | 0.0021 (6) | 0.0032 (6) | −0.0033 (6) |
| C7 | 0.0442 (9) | 0.0423 (9) | 0.0312 (8) | 0.0086 (7) | 0.0110 (7) | 0.0070 (6) |
| C5 | 0.0418 (9) | 0.0492 (10) | 0.0404 (9) | −0.0076 (8) | 0.0063 (7) | 0.0031 (7) |
| C1 | 0.0395 (8) | 0.0392 (9) | 0.0286 (8) | 0.0035 (7) | 0.0069 (6) | 0.0011 (6) |
| C8 | 0.0637 (13) | 0.0478 (11) | 0.0561 (12) | 0.0024 (9) | 0.0236 (10) | 0.0128 (9) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C6 | 1.3408 (18) | C4—H41 | 0.9500 |
| O1—C7 | 1.4544 (18) | C7—C8 | 1.496 (3) |
| O2—C6 | 1.2145 (18) | C7—H71 | 0.9900 |
| C3—C4 | 1.381 (2) | C7—H72 | 0.9900 |
| C3—C2 | 1.428 (2) | C5—H51 | 0.9800 |
| C3—C6 | 1.453 (2) | C5—H52 | 0.9800 |
| N1—C4 | 1.350 (2) | C5—H53 | 0.9800 |
| N1—C1 | 1.369 (2) | C1—H11 | 0.9500 |
| N1—H101 | 0.8800 | C8—H81 | 0.9800 |
| C2—C1 | 1.365 (2) | C8—H82 | 0.9800 |
| C2—C5 | 1.496 (2) | C8—H83 | 0.9800 |
| C6—O1—C7 | 116.25 (12) | O1—C7—H72 | 110.2 |
| C4—C3—C2 | 107.54 (13) | C8—C7—H72 | 110.2 |
| C4—C3—C6 | 125.81 (14) | H71—C7—H72 | 108.5 |
| C2—C3—C6 | 126.62 (13) | C2—C5—H51 | 109.5 |
| C4—N1—C1 | 109.53 (13) | C2—C5—H52 | 109.5 |
| C4—N1—H101 | 125.2 | H51—C5—H52 | 109.5 |
| C1—N1—H101 | 125.2 | C2—C5—H53 | 109.5 |
| C1—C2—C3 | 106.00 (13) | H51—C5—H53 | 109.5 |
| C1—C2—C5 | 126.62 (15) | H52—C5—H53 | 109.5 |
| C3—C2—C5 | 127.37 (13) | C2—C1—N1 | 109.07 (14) |
| O2—C6—O1 | 122.68 (14) | C2—C1—H11 | 125.5 |
| O2—C6—C3 | 124.38 (15) | N1—C1—H11 | 125.5 |
| O1—C6—C3 | 112.94 (12) | C7—C8—H81 | 109.5 |
| N1—C4—C3 | 107.85 (14) | C7—C8—H82 | 109.5 |
| N1—C4—H41 | 126.1 | H81—C8—H82 | 109.5 |
| C3—C4—H41 | 126.1 | C7—C8—H83 | 109.5 |
| O1—C7—C8 | 107.33 (14) | H81—C8—H83 | 109.5 |
| O1—C7—H71 | 110.2 | H82—C8—H83 | 109.5 |
| C8—C7—H71 | 110.2 | | |
| C4—C3—C2—C1 | 0.30 (17) | C2—C3—C6—O1 | 171.47 (13) |
| C6—C3—C2—C1 | 178.57 (14) | C1—N1—C4—C3 | −0.30 (17) |
| C4—C3—C2—C5 | 179.78 (15) | C2—C3—C4—N1 | 0.00 (17) |
| C6—C3—C2—C5 | −2.0 (3) | C6—C3—C4—N1 | −178.29 (14) |
| C7—O1—C6—O2 | −2.1 (2) | C6—O1—C7—C8 | 179.17 (13) |
| C7—O1—C6—C3 | 178.68 (12) | C3—C2—C1—N1 | −0.48 (17) |
| C4—C3—C6—O2 | 170.21 (15) | C5—C2—C1—N1 | −179.97 (15) |
| C2—C3—C6—O2 | −7.7 (2) | C4—N1—C1—C2 | 0.50 (17) |
| C4—C3—C6—O1 | −10.6 (2) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H101···O2$^{i}$ | 0.88 | 1.96 | 2.809 (2) | 163 |

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

**Fig. 1**

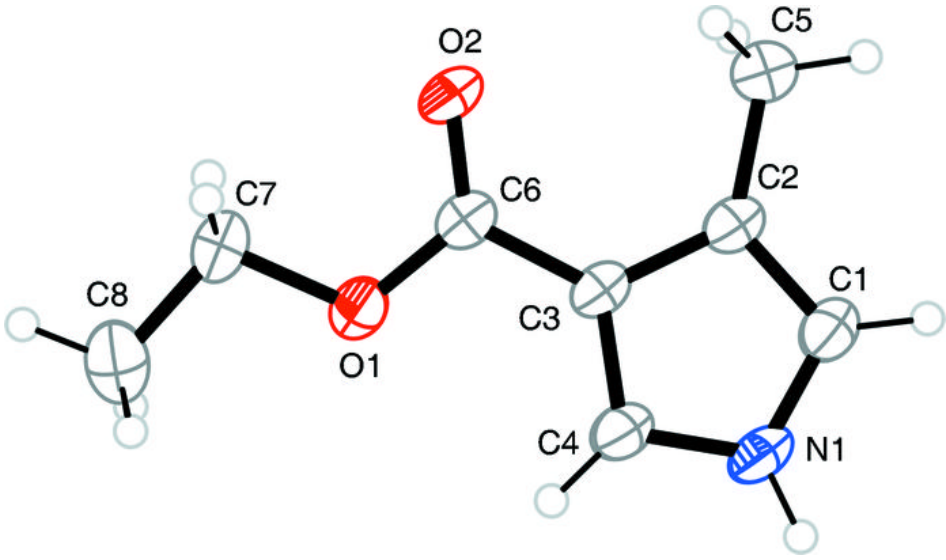

**Fig. 2**

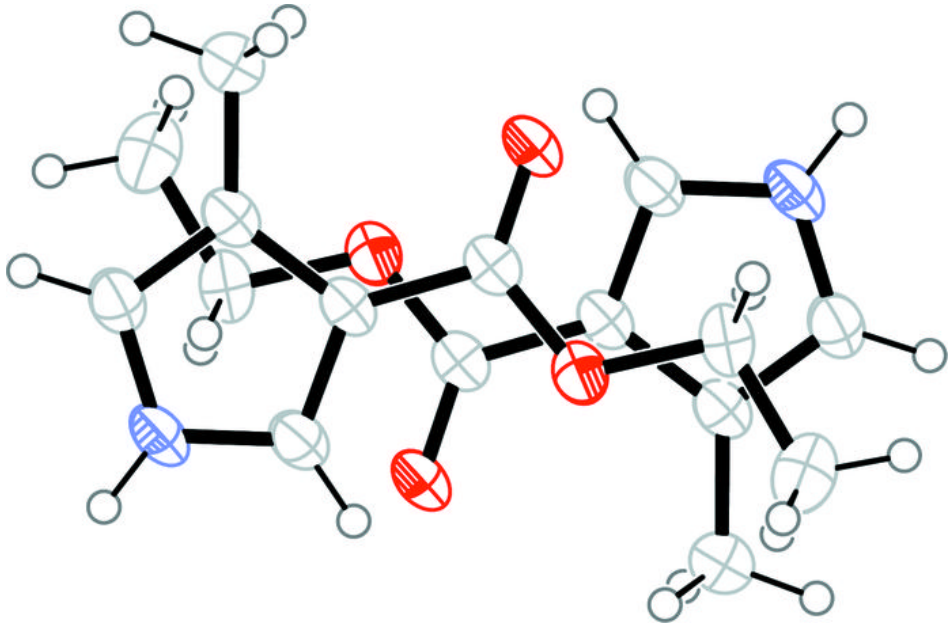

**Fig. 3**