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Ethyl 5-methyl-1*H*-pyrrole-2-carboxylate

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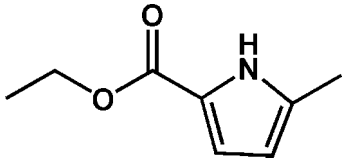
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.143; data-to-parameter ratio = 19.5.

In the title molecule, $C_8H_{11}NO_2$, the r.m.s. deviation of non-H atoms from their best plane is 0.031 Å. Molecules are connected *via* a pair of N—H···O hydrogen bonds into a centrosymmetric dimer.

Related literature

For the crystal structure of the 5-cyano analogue of the title compound, see: Zhang *et al.* (2003). For the synthesis of the title compound, see: Motekaitis *et al.* (1970).



Experimental

Crystal data

$C_8H_{11}NO_2$
M_r = 153.18
Monoclinic, $P2_1/c$
a = 7.0759 (3) Å
b = 18.0705 (9) Å
c = 6.6606 (3) Å
β = 101.349 (3)°
V = 835.01 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.20 × 0.15 × 0.13 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.984, T_{max} = 0.989
7496 measured reflections
1991 independent reflections
1157 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.143
S = 1.02
1991 reflections
102 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	1.99	2.8363 (19)	167

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2381).

References

Bruker (2007). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Motekaitis, R. J., Heinert, H. D. & Martell, A. E. (1970). *J. Org. Chem.* **35**, 2504–2511.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, Y.-H., Yin, Z., Li, X.-F., He, J. & Cheng, J.-P. (2003). *Acta Cryst.* E**59**, o1881–o1882.

supporting information

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Ethyl 5-methyl-1*H*-pyrrole-2-carboxylate

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S1. Comment

As part of our studies on hydrazone ligands bearing pyrrole unit the title compound was synthesized and characterized by X-ray diffraction.

The non-hydrogen atoms of the title molecule (Fig. 1) are situated in a fair plane (r.m.s. deviation of the non-hydrogen atoms being 0.0306 Å). In the crystal, the molecules are linked into a centrosymmetric dimer by two intermolecular N—H···O hydrogen bonds, forming a $R_2^2(10)$ ring motif (Table 1, Fig. 2).

S2. Experimental

The title compound was synthesized according to the literature procedure (Motekaitis *et al.*, 1970). The crude orange solid was washed well with ice water and dried in air. Colorless plates of the title compound were obtained by slow evaporation of petroleum ether/ethyl acetate (100:1) solution.

S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and were thereafter treated as riding, with U_{iso}(H) values of 1.5Ueq(C) for methyl groups and 1.2Ueq(C,*N*) for others.

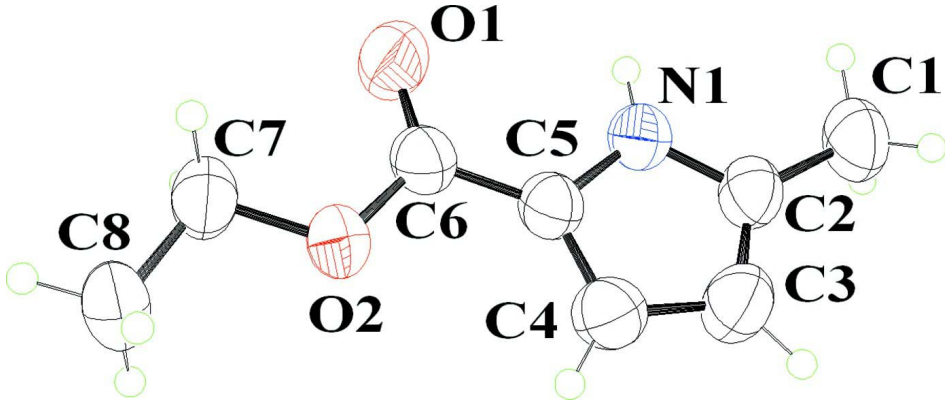

Figure 1

The title compound with the displacement ellipsoids shown at the 50% probability level.

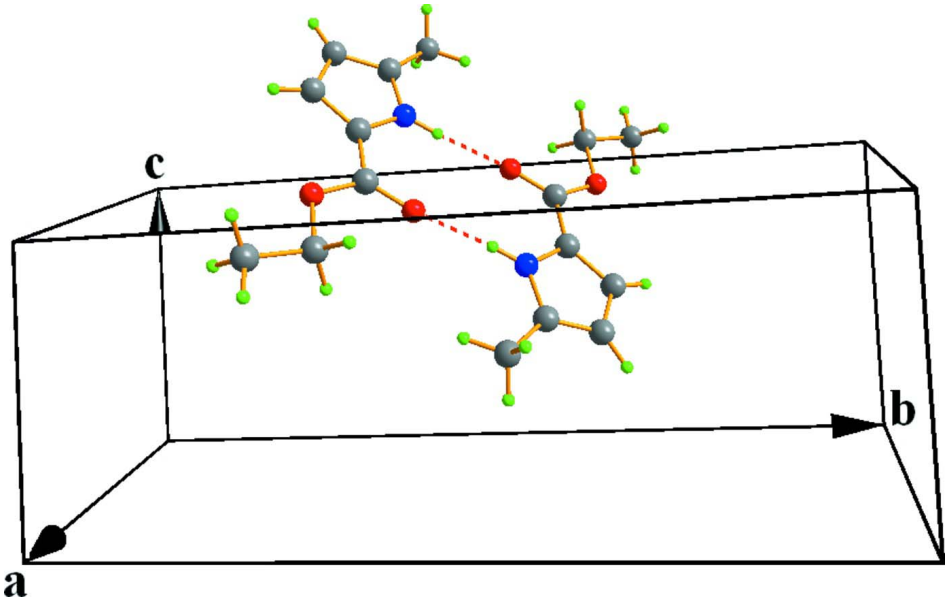

Figure 2

The centrosymmetric dimer *via* N-H···O hydrogen bonds of the title compound (hydrogen bonds shown as dashed lines, symmetry code:: 1 - *x*, 1 - *y*, 2 - *z*).

Ethyl 5-methyl-1*H*-pyrrole-2-carboxylate

Crystal data

$C_8H_{11}NO_2$
M_r = 153.18
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.0759 (3) Å
b = 18.0705 (9) Å
c = 6.6606 (3) Å
β = 101.349 (3)°
V = 835.01 (7) Å^3
Z = 4
$F(000)$ = 328
D_x = 1.218 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2070 reflections
θ = 2.3–24.2°
μ = 0.09 mm^{-1}
T = 296 K
Plate, colorless
0.20 × 0.15 × 0.13 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.984, T_{max} = 0.989
7496 measured reflections
1991 independent reflections
1157 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.9°, θ_{min} = 2.3°
h = −9→9
k = −23→23
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.143
S = 1.02
1991 reflections
102 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.0738P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.16$ e Å^{-3}
	$\Delta\rho_{min} = -0.16$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.12507 (16)	0.64959 (6)	0.92921 (18)	0.0629 (4)
N1	0.52408 (19)	0.57393 (7)	0.7402 (2)	0.0581 (4)
H1	0.5637	0.5360	0.8146	0.087*
C6	0.2631 (2)	0.60036 (9)	0.9187 (3)	0.0585 (4)
O1	0.2888 (2)	0.54602 (8)	1.0272 (2)	0.0861 (5)
C5	0.3729 (2)	0.61798 (9)	0.7644 (2)	0.0548 (4)
C2	0.6023 (2)	0.59835 (10)	0.5831 (3)	0.0600 (5)
C8	−0.1423 (3)	0.69326 (11)	1.0591 (3)	0.0768 (6)
H8A	−0.0794	0.7400	1.0916	0.115*
H8B	−0.2268	0.6837	1.1527	0.115*
H8C	−0.2159	0.6946	0.9217	0.115*
C4	0.3561 (2)	0.67196 (10)	0.6178 (3)	0.0651 (5)
H4	0.2658	0.7100	0.5976	0.078*
C7	0.0051 (3)	0.63353 (10)	1.0768 (3)	0.0691 (5)
H7A	0.0825	0.6324	1.2142	0.083*
H7B	−0.0569	0.5858	1.0480	0.083*
C1	0.7719 (3)	0.56133 (11)	0.5261 (3)	0.0780 (6)
H1A	0.8862	0.5893	0.5791	0.117*
H1B	0.7543	0.5585	0.3796	0.117*
H1C	0.7847	0.5123	0.5827	0.117*
C3	0.4987 (3)	0.65956 (10)	0.5044 (3)	0.0712 (5)
H3	0.5200	0.6879	0.3944	0.085*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0581 (7)	0.0624 (7)	0.0748 (8)	0.0073 (5)	0.0294 (6)	0.0035 (6)
N1	0.0533 (8)	0.0560 (8)	0.0691 (9)	0.0001 (6)	0.0221 (7)	0.0000 (6)
C6	0.0519 (9)	0.0563 (9)	0.0698 (11)	0.0019 (8)	0.0182 (8)	−0.0026 (9)
O1	0.0847 (10)	0.0820 (9)	0.1032 (11)	0.0273 (8)	0.0467 (8)	0.0332 (8)
C5	0.0486 (9)	0.0532 (9)	0.0649 (11)	−0.0015 (7)	0.0165 (8)	−0.0035 (8)

C2	0.0539 (9)	0.0652 (10)	0.0644 (11)	−0.0091 (8)	0.0202 (8)	−0.0063 (8)
C8	0.0689 (12)	0.0819 (13)	0.0884 (15)	0.0074 (10)	0.0373 (11)	−0.0054 (10)
C4	0.0587 (10)	0.0616 (10)	0.0766 (12)	0.0036 (8)	0.0172 (9)	0.0060 (9)
C7	0.0635 (11)	0.0788 (12)	0.0716 (12)	0.0050 (9)	0.0293 (9)	0.0048 (9)
C1	0.0664 (12)	0.0894 (14)	0.0867 (14)	−0.0022 (10)	0.0360 (10)	−0.0094 (11)
C3	0.0683 (11)	0.0781 (12)	0.0715 (12)	−0.0023 (10)	0.0246 (10)	0.0107 (10)

Geometric parameters (Å, º)

C2—C1	1.487 (2)	C1—H1A	0.9600
C2—C3	1.373 (3)	C1—H1B	0.9600
C4—C3	1.392 (2)	C1—H1C	0.9600
C5—C4	1.369 (2)	C3—H3	0.9300
N1—C2	1.351 (2)	C4—H4	0.9300
N1—C5	1.368 (2)	C7—H7A	0.9700
C6—C5	1.440 (2)	C7—H7B	0.9700
C6—O1	1.212 (2)	C8—H8A	0.9600
O2—C6	1.3333 (19)	C8—H8B	0.9600
O2—C7	1.4490 (19)	C8—H8C	0.9600
C8—C7	1.490 (2)	N1—H1	0.8600
C6—O2—C7	115.81 (13)	C5—C4—C3	107.57 (16)
C2—N1—C5	110.53 (14)	C5—C4—H4	126.2
C2—N1—H1	124.7	C3—C4—H4	126.2
C5—N1—H1	124.7	O2—C7—C8	107.22 (15)
O1—C6—O2	122.31 (15)	O2—C7—H7A	110.3
O1—C6—C5	124.50 (15)	C8—C7—H7A	110.3
O2—C6—C5	113.19 (15)	O2—C7—H7B	110.3
C4—C5—N1	106.89 (14)	C8—C7—H7B	110.3
C4—C5—C6	133.09 (16)	H7A—C7—H7B	108.5
N1—C5—C6	119.97 (15)	C2—C1—H1A	109.5
N1—C2—C3	106.81 (15)	C2—C1—H1B	109.5
N1—C2—C1	121.69 (16)	H1A—C1—H1B	109.5
C3—C2—C1	131.48 (17)	C2—C1—H1C	109.5
C7—C8—H8A	109.5	H1A—C1—H1C	109.5
C7—C8—H8B	109.5	H1B—C1—H1C	109.5
H8A—C8—H8B	109.5	C2—C3—C4	108.20 (16)
C7—C8—H8C	109.5	C2—C3—H3	125.9
H8A—C8—H8C	109.5	C4—C3—H3	125.9
H8B—C8—H8C	109.5		
C7—O2—C6—O1	−0.9 (2)	C5—N1—C2—C3	−0.1 (2)
C7—O2—C6—C5	177.93 (14)	C5—N1—C2—C1	178.73 (15)
C2—N1—C5—C4	−0.12 (19)	N1—C5—C4—C3	0.26 (19)
C2—N1—C5—C6	177.58 (14)	C6—C5—C4—C3	−177.02 (18)
O1—C6—C5—C4	173.57 (18)	C6—O2—C7—C8	−178.10 (14)
O2—C6—C5—C4	−5.3 (3)	N1—C2—C3—C4	0.2 (2)
O1—C6—C5—N1	−3.4 (3)	C1—C2—C3—C4	−178.40 (18)

O2—C6—C5—N1	177.75 (13)	C5—C4—C3—C2	−0.3 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	1.99	2.8363 (19)	167

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