Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl (2*E*)-2-cyano-3-(1-methyl-1*H*-pyrrol-2-yl)prop-2-enoate

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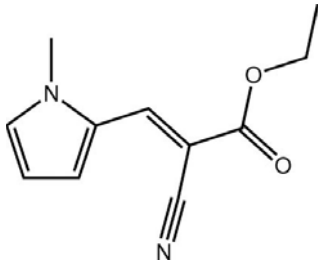
Received 6 August 2011; accepted 7 August 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.106; data-to-parameter ratio = 16.9.

The 15 non-H atoms of the title compound, $C_{11}H_{12}N_2O_2$, are approximately coplanar, the r.m.s. deviation being 0.145 Å. The major deviation from coplanarity is seen in a twist between the ethene (*E* configuration) and pyrrole rings [C—C—N—C torsion angle = −8.26 (18)°]. The carbonyl O and cyano N atoms are *syn* to each other. In the crystal, supramolecular linear tapes linked by C—H···O and C—H···N interactions are further connected by C—H···π(pyrrole) interactions.

Related literature

For background to the biological activity of 2(1*H*)pyridone compounds, see: Aly *et al.* (1991); Al-Saadi *et al.* (2005); Rostom *et al.* (2011).



Experimental

Crystal data

$C_{11}H_{12}N_2O_2$
M_r = 204.23
Triclinic, $P\overline{1}$
a = 7.6145 (3) Å
b = 8.4964 (6) Å
c = 9.7023 (6) Å
α = 64.898 (7)°
β = 89.859 (4)°
γ = 71.517 (5)°
V = 532.69 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.30 × 0.25 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.955, T_{max} = 1.000
4049 measured reflections
2336 independent reflections
1912 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.106
S = 1.04
2336 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

*Cg*1 is the centroid of the N2,C7—C10 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11a···O2^{i}	0.98	2.31	3.241 (2)	158
C9—H9···N1^{ii}	0.95	2.62	3.557 (2)	171
C11—H11b···*Cg*1^{iii}	0.98	2.69	3.5332 (17)	144

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6354).

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