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Ethyl 3-cyano-7-methylpyrazolo[1,5-*a*]-pyrimidine-6-carboxylate

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.105
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.

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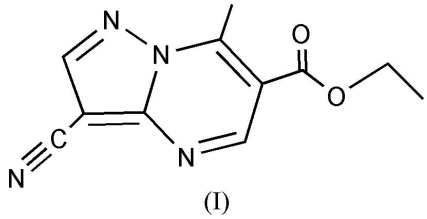
In the title molecule, $C_{11}H_{10}N_4O_2$, all bond lengths and angles are in normal ranges. In the crystal structure, weak intermolecular C—H···N hydrogen bonds link the molecules into centrosymmetric dimers. The crystal packing is further stabilized by van der Waals forces.

Comment

Pyrazolo[1,5-*a*]pyrimidine derivatives demonstrate various biological activities, *viz*. antibacterial, antischistosomal and xanthine oxidase inhibitor (Zoni *et al.*, 1998). Considerable interest has been focused on the synthesis of pyrazolo[1,5-*a*]pyrimidine derivatives *via* the versatile enaminones because of their synthetic and biological potential (Quiroga *et al.*, 1994). In a continuation of our study of structure–activity relationships in pyrazolo[1,5-*a*]pyrimidine derivatives (Wen *et al.*, 2004), we have synthesized the title compound, (I) (Fig. 1). We report its crystal structure here.



(I)

In the molecule, all bond lengths and angles are in normal ranges (Table 1). All atoms in the pyrazolopyrimidine moiety are essentially coplanar, the largest deviation from the mean plane being 0.016 (2) Å for atom C7. The pyrazole and pyrimidine rings make a dihedral angle of 1.01 (3)°, close to the value of 0.58° observed in ethyl 2-methylthio-7-phenyl-pyrazolo-[1,5-*a*]pyrimidine-3-carboxylate (Wen *et al.*, 2005). Weak intermolecular C—H···N hydrogen bonds (Table 2) link the molecules into centrosymmetric dimers. The crystal packing (Fig. 2) is further stabilized by van der Waals forces.

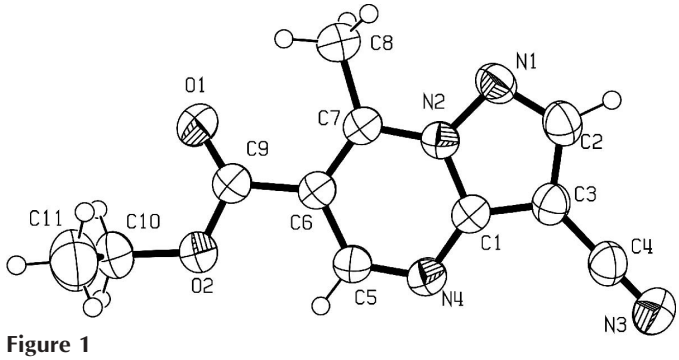


Figure 1
View of the title molecule, with 50% probability displacement ellipsoids.

Experimental

A mixture of ethyl 2-ethoxycarbonyl-3-dimethylamino-2-acrylate (3 mmol), 4-cyano-5-amino-1-*H*-pyrazole (3 mmol), and 20 ml glacial acetic acid in a 50 ml flask was stirred at room temperature for 4 h (monitored by TLC). The resulting solid product was filtered, washed with petroleum oil and dried. The pure product was isolated by recrystallization from ethanol; m.p. 374 K.

Crystal data

$C_{11}H_{10}N_4O_2$
M_r = 230.23
Monoclinic, $P2_1/c$
a = 6.8815 (11) Å
b = 16.468 (3) Å
c = 9.7901 (16) Å
β = 95.568 (2)°
V = 1104.2 (3) Å^3
Z = 4
D_x = 1.385 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2527 reflections
θ = 2.4–25.7°
μ = 0.10 mm^{-1}
T = 273 (2) K
Block, colourless
0.38 × 0.24 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.807, T_{max} = 0.980
5921 measured reflections
1943 independent reflections
1585 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.0°
$h = -8 \rightarrow 8$
$k = -18 \rightarrow 19$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.105
S = 1.05
1943 reflections
157 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.2206P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.058 (5)

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.322 (2)	C1—C3	1.386 (2)
N1—N2	1.3676 (17)	C2—C3	1.399 (2)
N2—C7	1.3627 (18)	C3—C4	1.417 (2)
N2—C1	1.3820 (18)	C5—C6	1.421 (2)
N4—C5	1.3127 (19)	C6—C7	1.375 (2)
N4—C1	1.344 (2)		
C2—N1—N2	103.61 (12)	N1—C2—C3	113.26 (14)
C7—N2—C1	122.92 (12)	C1—C3—C2	105.28 (13)
N1—N2—C1	112.77 (12)	N4—C5—C6	124.91 (14)
C5—N4—C1	115.30 (13)	C7—C6—C5	119.13 (13)
N4—C1—N2	122.51 (13)	N2—C7—C6	115.19 (12)
N2—C1—C3	105.08 (13)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···N3^{i}	0.97	2.58	3.384 (3)	141

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

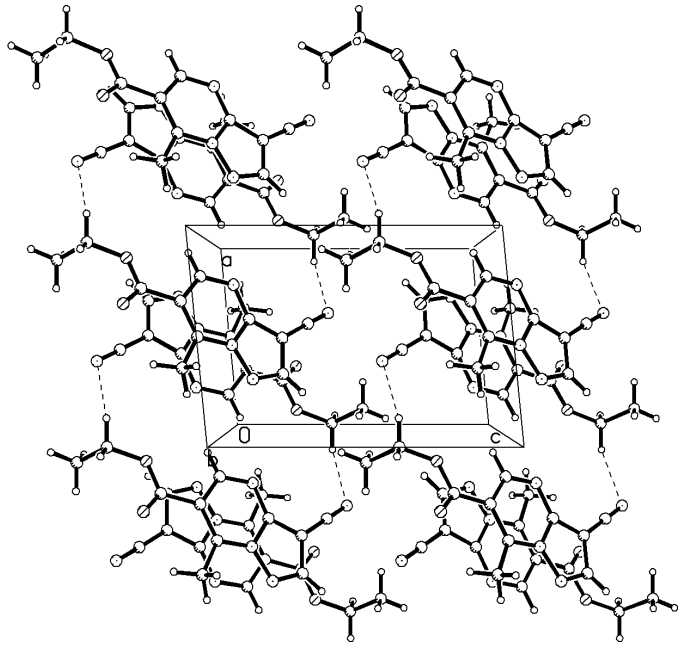


Figure 2
The crystal packing, viewed along the b axis. Intermolecular C—H···N hydrogen bonds are shown as dashed lines.

All H atoms were placed in calculated positions, with C—H = 0.93, 0.96 or 0.97 Å, and refined using a riding model, with U_{iso}(H) = 1.2 U_{eq}(C) for CH_2 and CH, and U_{iso}(H) = 1.5 U_{eq}(C) for CH_3.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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