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Methyl 1*H*-1,2,4-triazole-3-carboxylate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.111
Data-to-parameter ratio = 13.4

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

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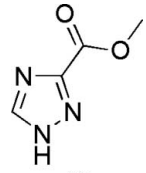
The title compound, $C_4H_5N_3O_2$, possesses a planar triazole ring and contains two intermolecular hydrogen bonds in the crystal structure.

Comment

Ribavirin (1-D-ribofuranosyl-1,2,4-triazole-3-carboxamide) (Vo *et al.*, 2003) is a nucleoside analogue that has demonstrated efficacy in treating viral diseases both as monotherapy 14 (respiratory syncytial virus) and in combination therapy with interferon alpha (hepatitis C virus). Methyl 1*H*-1,2,4-triazole-3-carboxylate, (I) (Lin & Liu, 1984), has been used as a starting material for ribavirin (Ramasamy *et al.*, 2000). The structure of (I) (Fig. 1) displays two types of intermolecular hydrogen-bonding interactions, O1···H1—C1 and N1···H3—N3. The plane-to-plane distance of two molecules is 3.26 (2) Å. Molecules lying in tha same plane are centrosymmetric and molecules in different planes are related by mirror symmetry.



(I)

Experimental

5-Amino-1,2,4-triazole-3-carboxylic acid (100 g) and methanol (500 ml) were placed in a 2 l three-necked flask with mechanical stirring. To the reaction mixture was slowly added 98% sulfuric acid (250 g) with stirring, and the mixture was heated under reflux for 16 h. The reaction mixture was cooled to 278 K for 10 h to afford a light-yellow wet solid. This solid was mixed with 98% sulfuric acid (58 g) and water (350 ml), and the resulting mixture cooled to 273–274 K. 30% aqueous sodium nitrite (150 g) was added slowly and the reaction allowed to continue for a further 2 h to give a grey solid. The grey solid and methanol (350 ml) were then placed in a 1 l flask with stirring and slowly heated to 313 K. When all the diazonium salt had been decomposed by methanol, the reaction solution was filtered and the filtrate was cooled to 283 K to afford the product, (I). Recrystallization from water and methanol gave 49 g of (I) (yield 49%).

Crystal data

$C_4H_5N_3O_2$
M_r = 127.11
Monoclinic, $P2_1/n$
a = 3.9737 (9) Å
b = 18.160 (4) Å
c = 8.1865 (19) Å
β = 102.596 (4)°
V = 576.5 (2) Å^3
Z = 4
D_x = 1.464 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1220 reflections
θ = 2.2–26.2°
μ = 0.12 mm^{-1}
T = 294 (2) K
Block, colourless
0.30 × 0.26 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.976
3192 measured reflections
1168 independent reflections
846 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.4°
$h = -2 \rightarrow 4$
$k = -22 \rightarrow 21$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.111
S = 1.04
1168 reflections
87 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2 + 0.0868P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C3	1.2008 (19)	N3—C1	1.318 (2)
N1—C1	1.323 (2)	N3—H3	0.95 (3)
N1—C2	1.353 (2)	C1—H1	0.9300
N2—C2	1.318 (2)	C4—H4*C*	0.9600
N2—N3	1.347 (2)		
C1—N3—H3	130.6 (15)	N1—C1—H1	124.8
N2—N3—H3	119.0 (15)	N1—C2—C3	121.13 (14)
N3—C1—H1	124.8	O2—C4—H4*A*	109.5
C2—N2—N3—C1	0.12 (18)	C1—N1—C2—C3	−179.58 (15)
C2—N1—C1—N3	0.14 (19)	N1—C2—C3—O1	3.1 (3)
N3—N2—C2—N1	−0.03 (18)	N1—C2—C3—O2	−176.59 (14)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1^{i}	0.93	2.57	3.138 (2)	120
N3—H3···N1^{i}	0.95 (3)	1.88 (3)	2.822 (2)	175 (2)

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

C-bound H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93 and 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C). The H atom bound to N3 was refined with the distance restraint N—H = 0.95 (3) Å.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

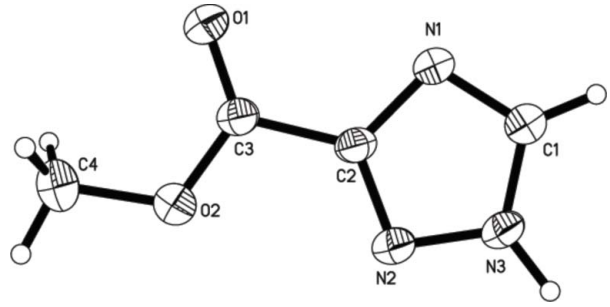


Figure 1
A view of the molecule of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

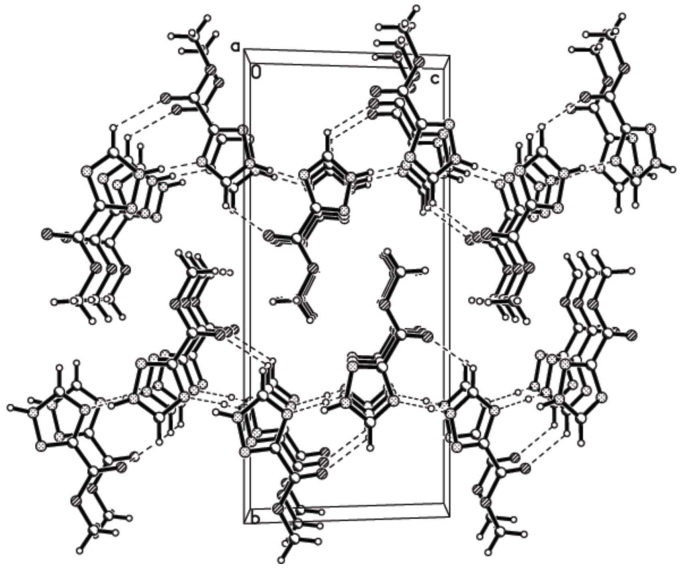


Figure 2
A packing diagram of (I). Dashed lines represent intermolecular hydrogen-bonding interactions.

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