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2-Ethoxymethyl-6-ethyl-2,3,4,5-tetrahydro-1,2,4-triazine-3,5-dione

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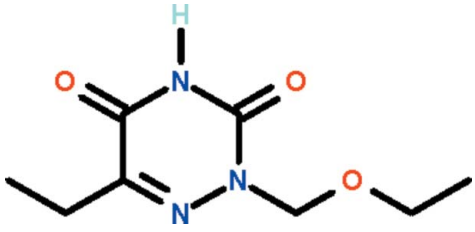
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.107; data-to-parameter ratio = 16.6.

The 1,2,4-triazine ring of the title compound, $C_8H_{13}N_3O_3$, is nearly planar (r.m.s. deviation = 0.019 Å). The imino group is hydrogen-bond donor to the exocyclic O atom at the 5-position of an adjacent molecule, the N—H···O hydrogen bond generating a chain parallel to the b axis.

Related literature

For the synthesis, see: El-Brollosy (2008).



Experimental

Crystal data

$C_8H_{13}N_3O_3$
M_r = 199.21
Monoclinic, $C2/c$
a = 20.4078 (19) Å
b = 4.4343 (3) Å
c = 22.6285 (17) Å
β = 111.813 (10)°
V = 1901.1 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 100 K
0.35 × 0.25 × 0.15 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.963, T_{max} = 0.984
3623 measured reflections
2174 independent reflections
1739 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
S = 1.06
2174 reflections
131 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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}	0.89 (2)	1.95 (2)	2.837 (2)	174.1 (17)

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5421).

References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
El-Brollosy, N. R. (2008). *Monatsh. Chem.* **139**, 1483–1490.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2012). E**68**, o346 [doi:10.1107/S1600536811055747]

2-Ethoxymethyl-6-ethyl-2,3,4,5-tetrahydro-1,2,4-triazine-3,5-dione

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S1. Comment

The compound (Scheme I) was synthesized for an evaluation of its anti-microbial properties (El-Brollosy, 2008). The 1,2,4-triazine ring is planar; the C atom at the 6-position deviates by 0.155 (2) Å from the mean plane whereas the C atom at the 2-position deviates from the mean plane by 0.081 (2) Å in the opposite direction (Fig. 1). The amino group is hydrogen-bond donor to the exocyclic O atom at the 5-position, the hydrogen bond generating a linear chain parallel to the *b*-axis of the monoclinc unit cell (Table 1, Fig. 2).

S2. Experimental

The compound was synthesized by using a reported method (El-Brollosy, 2008), and was recrystallized from ethanol.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H 0.95 to 0.98 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

The imino H-atom was located in a difference Fourier map, and was freely refined.

The -2 0 2 reflection that was affected by the beam-stop was omitted.

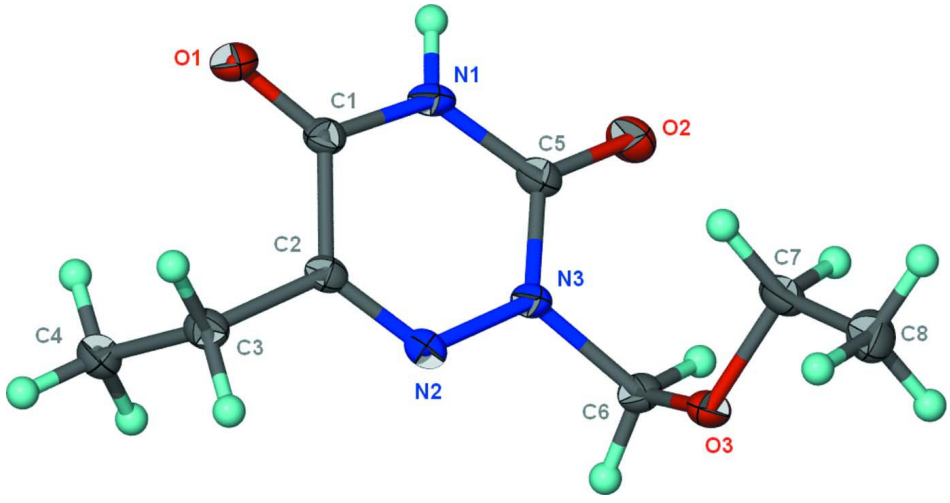

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_8H_{13}N_3O_3$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

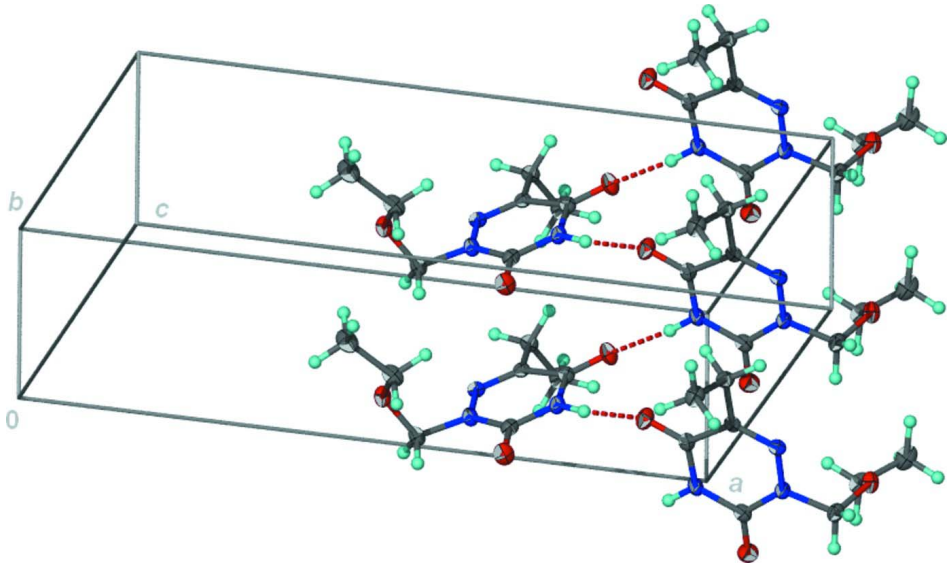

Figure 2

Hydrogen-bonded chain structure.

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Crystal data

$C_8H_{13}N_3O_3$
M_r = 199.21
Monoclinic, $C2/c$
Hall symbol: -C 2yc
a = 20.4078 (19) Å
b = 4.4343 (3) Å
c = 22.6285 (17) Å
β = 111.813 (10)°
V = 1901.1 (3) Å^3
Z = 8
$F(000)$ = 848
D_x = 1.392 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1592 reflections
θ = 2.3–27.5°
μ = 0.11 mm^{-1}
T = 100 K
Prism, colorless
0.35 × 0.25 × 0.15 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.963, T_{max} = 0.984
3623 measured reflections
2174 independent reflections
1739 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.6°, θ_{min} = 3.4°
h = −26→26
k = −5→5
l = −15→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.107
S = 1.06
2174 reflections
131 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 1.2698P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.73492 (5)	0.9252 (3)	0.68461 (5)	0.0201 (3)
O2	0.58065 (6)	0.2354 (3)	0.70746 (5)	0.0214 (3)
O3	0.42473 (5)	0.6126 (2)	0.59416 (5)	0.0172 (3)
N1	0.65902 (7)	0.5753 (3)	0.69639 (6)	0.0152 (3)
N2	0.56241 (6)	0.7358 (3)	0.57988 (6)	0.0138 (3)
N3	0.54722 (6)	0.5285 (3)	0.61778 (5)	0.0144 (3)
C1	0.67786 (7)	0.7953 (3)	0.66355 (7)	0.0141 (3)
C2	0.62375 (7)	0.8617 (3)	0.59987 (6)	0.0130 (3)
C3	0.64247 (8)	1.0709 (3)	0.55670 (7)	0.0159 (3)
H3A	0.6664	1.2510	0.5810	0.019*
H3B	0.5987	1.1387	0.5221	0.019*
C4	0.69101 (8)	0.9188 (4)	0.52750 (7)	0.0197 (3)
H4A	0.7019	1.0617	0.4994	0.030*
H4B	0.6672	0.7418	0.5029	0.030*
H4C	0.7349	0.8559	0.5616	0.030*
C5	0.59417 (8)	0.4319 (3)	0.67624 (7)	0.0152 (3)
C6	0.47519 (8)	0.4069 (3)	0.59096 (7)	0.0167 (3)
H6A	0.4642	0.3508	0.5459	0.020*
H6B	0.4726	0.2216	0.6144	0.020*
C7	0.42810 (8)	0.6726 (4)	0.65804 (7)	0.0200 (3)
H7A	0.4709	0.7914	0.6818	0.024*
H7B	0.4300	0.4809	0.6810	0.024*
C8	0.36268 (9)	0.8478 (4)	0.65258 (8)	0.0252 (4)
H8A	0.3635	0.8925	0.6953	0.038*
H8B	0.3207	0.7277	0.6292	0.038*
H8C	0.3614	1.0369	0.6298	0.038*
H1	0.6913 (10)	0.515 (4)	0.7331 (9)	0.024 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0179 (6)	0.0261 (6)	0.0138 (5)	−0.0056 (5)	0.0028 (4)	−0.0018 (4)
O2	0.0237 (6)	0.0226 (6)	0.0166 (5)	−0.0020 (5)	0.0059 (4)	0.0063 (5)
O3	0.0153 (5)	0.0246 (6)	0.0112 (5)	0.0001 (5)	0.0043 (4)	−0.0008 (4)
N1	0.0148 (6)	0.0179 (7)	0.0095 (6)	0.0019 (5)	0.0007 (5)	0.0013 (5)
N2	0.0168 (6)	0.0133 (6)	0.0118 (6)	0.0010 (5)	0.0059 (5)	0.0008 (5)
N3	0.0141 (6)	0.0171 (6)	0.0102 (6)	−0.0017 (5)	0.0026 (5)	0.0019 (5)
C1	0.0146 (7)	0.0161 (7)	0.0115 (7)	0.0006 (6)	0.0047 (5)	−0.0019 (6)
C2	0.0153 (7)	0.0126 (7)	0.0110 (7)	0.0019 (6)	0.0048 (5)	−0.0006 (6)
C3	0.0183 (7)	0.0149 (7)	0.0138 (7)	−0.0010 (6)	0.0049 (6)	0.0006 (6)

C4	0.0205 (8)	0.0245 (8)	0.0153 (7)	−0.0030 (7)	0.0081 (6)	−0.0011 (6)
C5	0.0171 (7)	0.0163 (7)	0.0121 (7)	0.0027 (6)	0.0054 (6)	0.0001 (6)
C6	0.0159 (7)	0.0188 (8)	0.0141 (7)	−0.0035 (6)	0.0039 (6)	−0.0015 (6)
C7	0.0246 (8)	0.0243 (8)	0.0118 (7)	−0.0063 (7)	0.0075 (6)	−0.0017 (6)
C8	0.0254 (9)	0.0310 (9)	0.0226 (8)	−0.0068 (8)	0.0127 (7)	−0.0089 (7)

Geometric parameters (Å, º)

O1—C1	1.2256 (18)	C3—H3A	0.9900
O2—C5	1.2164 (18)	C3—H3B	0.9900
O3—C6	1.3974 (18)	C4—H4A	0.9800
O3—C7	1.4461 (17)	C4—H4B	0.9800
N1—C1	1.3654 (19)	C4—H4C	0.9800
N1—C5	1.3839 (19)	C6—H6A	0.9900
N1—H1	0.889 (19)	C6—H6B	0.9900
N2—C2	1.2894 (19)	C7—C8	1.509 (2)
N2—N3	1.3688 (16)	C7—H7A	0.9900
N3—C5	1.3821 (18)	C7—H7B	0.9900
N3—C6	1.4686 (19)	C8—H8A	0.9800
C1—C2	1.4832 (19)	C8—H8B	0.9800
C2—C3	1.496 (2)	C8—H8C	0.9800
C3—C4	1.536 (2)		
C6—O3—C7	114.18 (11)	H4A—C4—H4C	109.5
C1—N1—C5	125.26 (13)	H4B—C4—H4C	109.5
C1—N1—H1	117.7 (12)	O2—C5—N3	123.49 (14)
C5—N1—H1	117.0 (12)	O2—C5—N1	122.24 (13)
C2—N2—N3	119.17 (12)	N3—C5—N1	114.26 (13)
N2—N3—C5	124.75 (12)	O3—C6—N3	112.50 (12)
N2—N3—C6	114.37 (11)	O3—C6—H6A	109.1
C5—N3—C6	120.88 (12)	N3—C6—H6A	109.1
O1—C1—N1	122.90 (13)	O3—C6—H6B	109.1
O1—C1—C2	122.78 (13)	N3—C6—H6B	109.1
N1—C1—C2	114.33 (12)	H6A—C6—H6B	107.8
N2—C2—C1	122.02 (13)	O3—C7—C8	107.51 (12)
N2—C2—C3	119.31 (12)	O3—C7—H7A	110.2
C1—C2—C3	118.61 (13)	C8—C7—H7A	110.2
C2—C3—C4	111.76 (12)	O3—C7—H7B	110.2
C2—C3—H3A	109.3	C8—C7—H7B	110.2
C4—C3—H3A	109.3	H7A—C7—H7B	108.5
C2—C3—H3B	109.3	C7—C8—H8A	109.5
C4—C3—H3B	109.3	C7—C8—H8B	109.5
H3A—C3—H3B	107.9	H8A—C8—H8B	109.5
C3—C4—H4A	109.5	C7—C8—H8C	109.5
C3—C4—H4B	109.5	H8A—C8—H8C	109.5
H4A—C4—H4B	109.5	H8B—C8—H8C	109.5
C3—C4—H4C	109.5		

C2—N2—N3—C5	−2.5 (2)	C1—C2—C3—C4	74.86 (17)
C2—N2—N3—C6	178.28 (12)	N2—N3—C5—O2	−175.83 (13)
C5—N1—C1—O1	176.71 (14)	C6—N3—C5—O2	3.3 (2)
C5—N1—C1—C2	−4.0 (2)	N2—N3—C5—N1	3.3 (2)
N3—N2—C2—C1	−1.8 (2)	C6—N3—C5—N1	−177.56 (12)
N3—N2—C2—C3	175.47 (12)	C1—N1—C5—O2	179.42 (14)
O1—C1—C2—N2	−175.88 (14)	C1—N1—C5—N3	0.3 (2)
N1—C1—C2—N2	4.8 (2)	C7—O3—C6—N3	−68.72 (15)
O1—C1—C2—C3	6.9 (2)	N2—N3—C6—O3	−74.79 (15)
N1—C1—C2—C3	−172.48 (12)	C5—N3—C6—O3	106.00 (15)
N2—C2—C3—C4	−102.47 (16)	C6—O3—C7—C8	−169.27 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.89 (2)	1.95 (2)	2.837 (2)	174.1 (17)

Symmetry code: (i) −*x*+3/2, *y*−1/2, −*z*+3/2.