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Methyl 5-(1-benzofuran-2-yl)isoxazole-3-carboxylate

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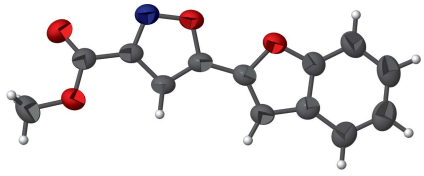
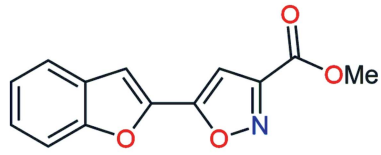
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{13}H_9NO_4$, is almost planar (r.m.s. deviation = 0.071 Å). In the crystal, weak C—H···O and C—H···N interactions connect the molecules into ribbons propagating parallel to the *a*-axis direction.

3D view



Chemical scheme



Structure description

Compounds containing a benzofuran ring system show interesting pharmaceutical applications (Khanam & Shamsuzzaman, 2015; Dawood, 2013). As part of our studies in this area, we now describe the crystal structure of the title compound.

Apart from the methyl hydrogen atoms, the molecule (Fig. 1) is almost planar [dihedral angle between the ring systems = 0.27 (9)°; r.m.s. deviation for the non-hydrogen atoms = 0.071 Å]. In the crystal, weak C—H···O and extremely weak C—H···N interactions form ribbons running parallel to [100] (Table 1, Fig. 2) with adjacent molecules in the chain related by *a*-glide symmetry.

Synthesis and crystallization

The title compound was synthesized based on a literature procedure (Siddiqui *et al.*, 2013) and recrystallized from dimethylformamide solution to yield colourless block-shaped crystals.

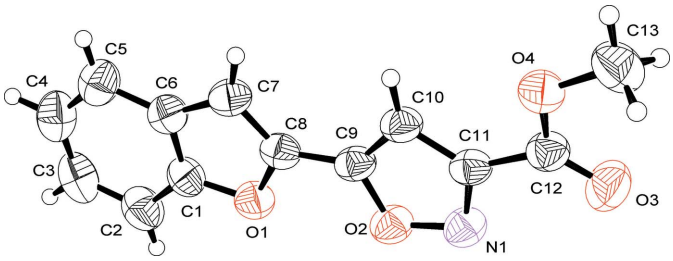


Figure 1
The molecular structure showing 50% displacement ellipsoids.

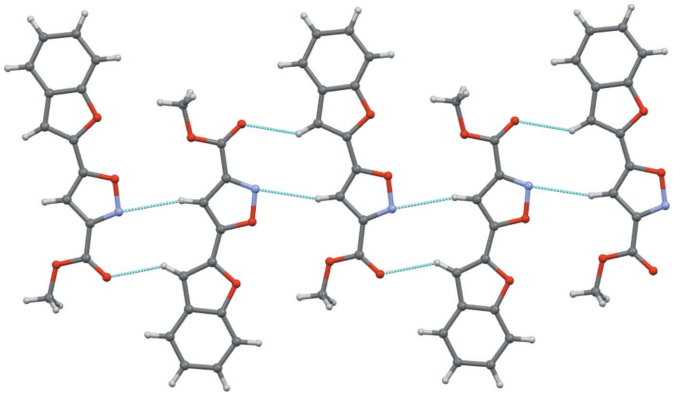


Figure 2
Intermolecular interactions forming a ribbon along the *a*-axis.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O3^{i}	0.93	2.47	3.248 (3)	142
C10—H10···N1^{i}	0.93	2.69	3.600 (2)	165

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_9NO_4$
M_r	243.21
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	296
a, b, c (Å)	11.5170 (6), 8.7431 (4), 22.2595 (13)
V (Å^3)	2241.4 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.29 × 0.24 × 0.20
Data collection	
Diffractometer	Agilent SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.993, 0.995
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7841, 2754, 1729
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.693
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.128, 1.04
No. of reflections	2754
No. of parameters	164
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.18

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS2013* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

full crystallographic data

IUCrData (2017). **2**, x171820 [https://doi.org/10.1107/S241431461701820X]

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Methyl 5-(1-benzofuran-2-yl)isoxazole-3-carboxylate

Crystal data

$C_{13}H_9NO_4$
M_r = 243.21
Orthorhombic, *Pbca*
a = 11.5170 (6) Å
b = 8.7431 (4) Å
c = 22.2595 (13) Å
V = 2241.4 (2) Å^3
Z = 8
F(000) = 1008
D_x = 1.441 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2289 reflections
θ = 4.7–27.2°
μ = 0.11 mm^{-1}
T = 296 K
Block, colourless
0.29 × 0.24 × 0.20 mm

Data collection

Agilent SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.993, T_{max} = 0.995
7841 measured reflections
2754 independent reflections
1729 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 29.5°, θ_{min} = 3.5°
h = −15→11
k = −8→11
l = −30→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.128
S = 1.04
2754 reflections
164 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.7049P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Special details

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

Refinement. All hydrogen atoms were placed in calculated positions and refined using a riding model. Methyl C—H bonds were fixed at 0.96 Å, with displacement parameters 1.5 times U_{eq}(C), and were allowed to spin about the C—C bond. Aromatic C—H distances were set to 0.93 Å and their U(iso) set to 1.2 times the U_{eq} for the atoms to which they are bonded.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.67167 (18)	0.3721 (2)	0.65576 (8)	0.0537 (5)
C2	0.7252 (2)	0.2758 (3)	0.69597 (10)	0.0708 (6)
H2	0.8055	0.2638	0.6967	0.085*
C3	0.6540 (3)	0.1981 (3)	0.73512 (10)	0.0758 (7)
H3	0.6866	0.1318	0.7631	0.091*
C4	0.5339 (2)	0.2169 (3)	0.73359 (11)	0.0730 (6)
H4	0.4880	0.1625	0.7605	0.088*
C5	0.4817 (2)	0.3140 (2)	0.69324 (10)	0.0655 (6)
H5	0.4015	0.3260	0.6927	0.079*
C6	0.55252 (17)	0.3945 (2)	0.65298 (9)	0.0521 (5)
C7	0.53436 (16)	0.5028 (2)	0.60614 (9)	0.0527 (5)
H7	0.4634	0.5416	0.5932	0.063*
C8	0.63964 (16)	0.5379 (2)	0.58428 (8)	0.0490 (4)
C9	0.67308 (15)	0.6425 (2)	0.53750 (8)	0.0480 (4)
C10	0.61160 (16)	0.7336 (2)	0.50057 (8)	0.0501 (4)
H10	0.5314	0.7451	0.4988	0.060*
C11	0.69573 (15)	0.8071 (2)	0.46541 (8)	0.0475 (4)
C12	0.67921 (17)	0.9195 (2)	0.41622 (9)	0.0527 (5)
C13	0.5415 (2)	1.0774 (3)	0.36919 (10)	0.0745 (6)
H13A	0.5791	1.1724	0.3785	0.112*
H13B	0.4589	1.0925	0.3682	0.112*
H13C	0.5674	1.0416	0.3307	0.112*
N1	0.80140 (13)	0.76549 (19)	0.47946 (8)	0.0568 (4)
O1	0.72689 (11)	0.45958 (15)	0.61324 (6)	0.0565 (4)
O2	0.78819 (10)	0.65920 (15)	0.52603 (6)	0.0570 (4)
O3	0.75434 (14)	0.96214 (19)	0.38300 (7)	0.0768 (5)
O4	0.56996 (11)	0.96551 (16)	0.41459 (6)	0.0610 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0607 (12)	0.0534 (11)	0.0471 (10)	0.0046 (9)	−0.0011 (9)	−0.0067 (9)
C2	0.0727 (15)	0.0787 (15)	0.0612 (13)	0.0129 (12)	−0.0069 (11)	0.0009 (12)
C3	0.105 (2)	0.0684 (14)	0.0541 (12)	0.0145 (14)	−0.0020 (13)	0.0021 (11)
C4	0.0961 (19)	0.0607 (13)	0.0621 (13)	−0.0018 (13)	0.0144 (13)	−0.0011 (11)
C5	0.0709 (14)	0.0580 (11)	0.0675 (13)	−0.0009 (11)	0.0119 (11)	−0.0039 (11)
C6	0.0546 (12)	0.0479 (10)	0.0538 (11)	0.0014 (9)	0.0025 (9)	−0.0097 (9)
C7	0.0442 (10)	0.0515 (10)	0.0625 (12)	0.0028 (8)	−0.0015 (9)	−0.0038 (9)
C8	0.0461 (10)	0.0496 (10)	0.0512 (10)	0.0041 (8)	−0.0043 (8)	−0.0075 (9)
C9	0.0387 (9)	0.0517 (10)	0.0537 (10)	−0.0005 (8)	0.0020 (8)	−0.0108 (9)

C10	0.0369 (9)	0.0585 (11)	0.0548 (10)	0.0005 (8)	−0.0005 (8)	−0.0049 (9)
C11	0.0399 (10)	0.0503 (10)	0.0522 (10)	0.0007 (8)	0.0006 (8)	−0.0104 (9)
C12	0.0486 (11)	0.0568 (11)	0.0526 (11)	−0.0025 (9)	0.0015 (9)	−0.0069 (9)
C13	0.0792 (16)	0.0744 (14)	0.0698 (14)	0.0081 (12)	−0.0176 (12)	0.0078 (12)
N1	0.0444 (9)	0.0608 (10)	0.0651 (10)	0.0012 (8)	0.0038 (8)	0.0006 (9)
O1	0.0463 (8)	0.0653 (8)	0.0579 (8)	0.0054 (6)	−0.0023 (6)	0.0010 (7)
O2	0.0407 (7)	0.0623 (8)	0.0680 (9)	0.0049 (6)	0.0003 (6)	0.0019 (7)
O3	0.0590 (9)	0.0931 (12)	0.0782 (10)	−0.0027 (8)	0.0141 (8)	0.0173 (9)
O4	0.0492 (8)	0.0714 (9)	0.0625 (8)	0.0041 (7)	−0.0041 (6)	0.0062 (7)

Geometric parameters (Å, º)

C1—O1	1.373 (2)	C8—C9	1.438 (3)
C1—C2	1.375 (3)	C9—C10	1.346 (3)
C1—C6	1.388 (3)	C9—O2	1.358 (2)
C2—C3	1.377 (3)	C10—C11	1.402 (3)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.393 (4)	C11—N1	1.308 (2)
C3—H3	0.9300	C11—C12	1.483 (3)
C4—C5	1.375 (3)	C12—O3	1.198 (2)
C4—H4	0.9300	C12—O4	1.322 (2)
C5—C6	1.401 (3)	C13—O4	1.444 (2)
C5—H5	0.9300	C13—H13A	0.9600
C6—C7	1.424 (3)	C13—H13B	0.9600
C7—C8	1.342 (3)	C13—H13C	0.9600
C7—H7	0.9300	N1—O2	1.401 (2)
C8—O1	1.376 (2)		
O1—C1—C2	125.59 (19)	O1—C8—C9	117.38 (16)
O1—C1—C6	110.40 (16)	C10—C9—O2	109.58 (16)
C2—C1—C6	124.0 (2)	C10—C9—C8	132.65 (17)
C1—C2—C3	116.5 (2)	O2—C9—C8	117.77 (16)
C1—C2—H2	121.7	C9—C10—C11	104.40 (16)
C3—C2—H2	121.7	C9—C10—H10	127.8
C2—C3—C4	121.2 (2)	C11—C10—H10	127.8
C2—C3—H3	119.4	N1—C11—C10	112.46 (17)
C4—C3—H3	119.4	N1—C11—C12	118.69 (17)
C5—C4—C3	121.6 (2)	C10—C11—C12	128.85 (17)
C5—C4—H4	119.2	O3—C12—O4	125.17 (19)
C3—C4—H4	119.2	O3—C12—C11	124.70 (19)
C4—C5—C6	118.3 (2)	O4—C12—C11	110.13 (16)
C4—C5—H5	120.9	O4—C13—H13A	109.5
C6—C5—H5	120.9	O4—C13—H13B	109.5
C1—C6—C5	118.43 (19)	H13A—C13—H13B	109.5
C1—C6—C7	105.78 (17)	O4—C13—H13C	109.5
C5—C6—C7	135.8 (2)	H13A—C13—H13C	109.5
C8—C7—C6	106.55 (17)	H13B—C13—H13C	109.5
C8—C7—H7	126.7	C11—N1—O2	105.10 (14)

C6—C7—H7	126.7	C1—O1—C8	105.19 (14)
C7—C8—O1	112.08 (17)	C9—O2—N1	108.46 (13)
C7—C8—C9	130.53 (17)	C12—O4—C13	116.21 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O3^{i}	0.93	2.47	3.248 (3)	142
C10—H10···N1^{i}	0.93	2.69	3.600 (2)	165

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