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1-(Prop-2-ynyl)-1*H*-benzimidazol-2(3*H*)-one

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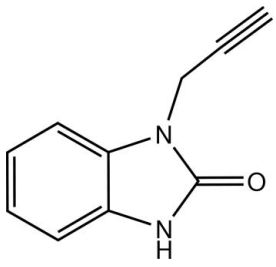
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.101; data-to-parameter ratio = 17.5.

The benzimidazolone part of the title molecule, $C_{10}H_8N_2O$, is almost planar [r.m.s. deviation = 0.014 (1) Å] and the $NCH_2C{\equiv}CH$ group forms a dihedral angle of 67.95 (6)° with its best plane. In the crystal, molecules form inversion dimers *via* pairs of N—H···O hydrogen bonds. C—H···O interactions connect the dimers, forming a two-dimensional polymeric network parallel to (100).

Related literature

For pharmacological and biochemical properties of benzimidazole dirivatives, see: Gravatt *et al.* (1994); Horton *et al.* (2003); Kim *et al.* (1996); Roth *et al.* (1997). For similar structures, see: Ouzidan, Kandri Rodi, Butcher*et al.* (2011); Ouzidan, Kandri Rodi, Fronczek *et al.* (2011); Ouzidan, Kandri Rodi, Jasinski *et al.* (2011); Belaziz *et al.* (2012).



Experimental

Crystal data

$C_{10}H_8N_2O$ M_r = 172.18
Monoclinic, $P2_1/c$
a = 4.5553 (6) Å
b = 18.001 (3) Å
c = 10.7488 (13) Å
β = 93.645 (8)°
V = 879.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.41 × 0.32 × 0.15 mm

Data collection

Bruker X8 APEXII diffractometer
10826 measured reflections
2080 independent reflections
1753 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.101
S = 1.05
2080 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 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}	0.95	1.88	2.8226 (12)	174
C10—H10···O1^{ii}	0.96	2.39	3.2541 (17)	149

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2546).

References

Belaziz, D., Kandri Rodi, Y., Ouazzani Chahdi, F., Essassi, E. M., Saadi, M. & El Ammari, L. (2012). *Acta Cryst.* E**68**, o3212.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Gravatt, G. L., Baguley, B. C., Wilson, W. R. & Denny, W. A. (1994). *J. Med. Chem.* **37**, 4338–4345.
Horton, D. A., Bourne, G. T. & Smythe, M. L. (2003). *Chem. Rev.* **103**, 893–930.
Kim, J. S., Gatto, B., Yu, C., Liu, A., Liu, L. F. & La Voie, E. J. (1996). *J. Med. Chem.* **39**, 992–998.
Ouzidan, Y., Kandri Rodi, Y., Butcher, R. J., Essassi, E. M. & El Ammari, L. (2011). *Acta Cryst.* E**67**, o283.
Ouzidan, Y., Kandri Rodi, Y., Fronczek, F. R., Venkatraman, R., El Ammari, L. & Essassi, E. M. (2011). *Acta Cryst.* E**67**, o362–o363.
Ouzidan, Y., Kandri Rodi, Y., Jasinski, J. P., Butcher, R. J., Golen, J. A. & El Ammari, L. (2011). *Acta Cryst.* E**67**, o1091.
Roth, T., Morningstar, M. L., Boyer, P. L., Hughes, S. H., Buckheit, R. W. & Michejda, C. J. (1997). *J. Med. Chem.* **40**, 4199–4207.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

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Acta Cryst. (2013). E**69**, o119 [https://doi.org/10.1107/S160053681205088X]

1-(Prop-2-ynyl)-1*H*-benzimidazol-2(3*H*)-one

Younès Ouzidan, Youssef Kandri Rodi, Fouad Ouazzani Chahdi, El Mokhtar Essassi, Mohamed Saadi and Lahcen El Ammari

S1. Comment

Benzimidazoles are very useful intermediates/subunits for the development of molecules of pharmaceutical or biological interest. Benzimidazole and its derivatives are an important class of bioactive molecules in the field of drugs and pharmaceuticals. Benzimidazole derivatives have found applications in diverse therapeutic areas including anti-ulcers, anti-hypertensives, anti-virals, anti-fungals, anti-cancers, (Gravatt *et al.*, 1994; Horton *et al.*, 2003; Kim *et al.*, 1996; Roth *et al.*, 1997).

As a continuation of our research work devoted to the development of substituted benzimidazol-2-one derivatives (Ouzidan, Kandri Rodi, Butcher *et al.*, 2011; Ouzidan, Kandri Rodi, Fronczek *et al.*, 2011; Belaziz *et al.* 2012), we reported in this paper the synthesis of benzimidazol-2-one derivative by action of propargyl bromide with 1*H*-benzo[*d*]imidazol-2(3*H*)-one in the presence of a catalytic quantity of tetra-n-butylammonium bromide under mild conditions to furnish two compounds: di-substituted (Ouzidan, Kandri Rodi, Jasinski *et al.*, 2011) and mono-substituted (Scheme 1).

The two fused five- and six-membered rings building the molecule of the title compound, $C_{10}H_8N_2O$, are approximately planar, the largest deviation from the mean plane being 0.014 (2) Å at C1 (Fig.1). The C1–N2–C8–C9 torsion angle along the bond between the benzimidazolone and the prop-2-ynyl groups is -109.99 (12)°. In the crystal, the molecules form centrosymmetric cyclic dimers via a pair of N1–H1···O1 hydrogen-bonds (Fig.2 and Table2). In addition, intermolecular C10–H10···O1 interaction beteen the acetylenic H atom and the carbonyl O atom connects the dimers into (100) layers.

S2. Experimental

To 1*H*-benzo[*d*]imidazol-2(3*H*)-one (0.2 g, 1.5 mmol), potassium carbonate (0.41 g, 3 mmol) and tetra-n-butyl-ammonium bromide (0.05 g, 0.15 mmol) in DMF (15 ml) was added propargyl bromide (0.16 ml, 1.8 mmol). Stirring was continued at room temperature for 6 h. The salt was removed by filtration and the filtrate concentrated under reduced pressure. The residue was separated by chromatography on a column of silica gel with ethyl acetate/petroleum ether (1/2) as eluent. Colourless crystals were isolated when the solvent was allowed to evaporate (m.p. 399 K).

S3. Refinement

All H atoms could be located in a difference Fourier map. However, they were placed in calculated positions with N—H = 0.86 Å, C—H = 0.93 Å (aromatic), and C—H = 0.97 Å (methylene) and refined as riding on their parent atoms with U_{iso}(H) = 1.2 U_{eq} (C, N).

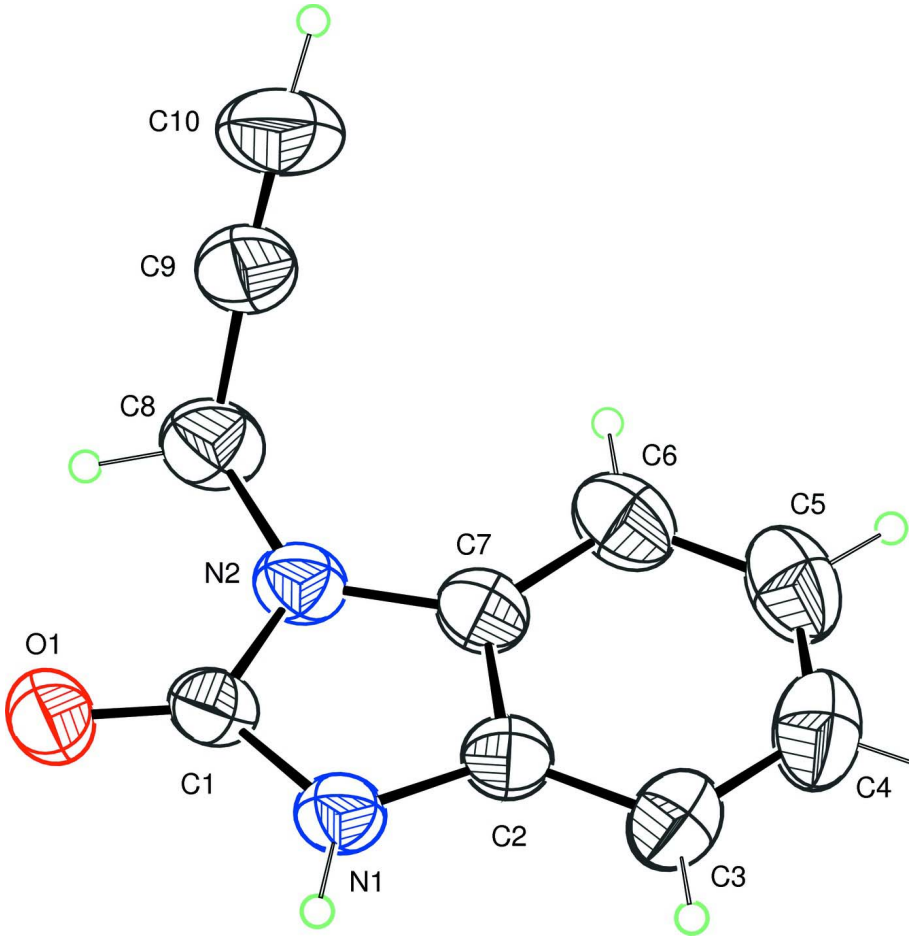

Figure 1

Molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles.

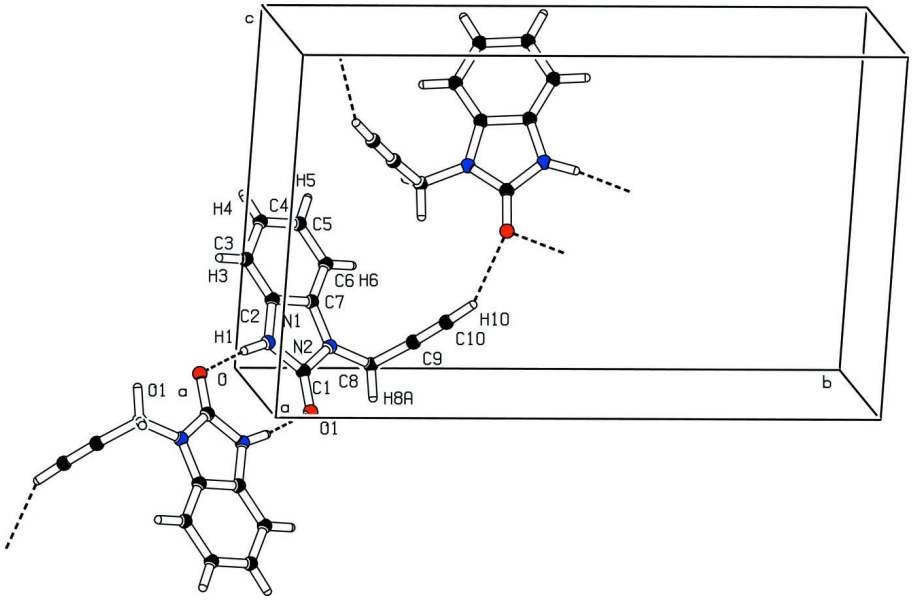

Figure 2

Intermolecular interactions in the title compound. Hydrogen bonds are shown as dashed lines. Symmetry codes: (i) -*x* + 1, -*y* + 1, -*z* + 1; (ii) *x*, -*y* + 1/2, *z* + 1/2.

1-(Prop-2-ynyl)-1*H*-benzimidazol-2(3*H*)-one

Crystal data

$C_{10}H_8N_2O$
M_r = 172.18
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 4.5553 (6) Å
b = 18.001 (3) Å
c = 10.7488 (13) Å
β = 93.645 (8)°
V = 879.6 (2) Å^3
Z = 4
$F(000)$ = 360
D_x = 1.300 Mg m^{-3}
Melting point: 399 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2080 reflections
θ = 3.0–27.9°
μ = 0.09 mm^{-1}
T = 296 K
Block, colourless
0.41 × 0.32 × 0.15 mm

Data collection

Bruker X8 APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
10826 measured reflections
2080 independent reflections
1753 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.9°, θ_{min} = 3.0°
h = −5→5
k = −23→23
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.101
S = 1.05
2080 reflections
119 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.1197P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.018 (4)

Special details

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

Refinement. Refinement of F^2 against all reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on all data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.43254 (19)	0.40104 (4)	0.43888 (7)	0.0527 (2)
N1	0.25564 (19)	0.46700 (5)	0.60486 (8)	0.0425 (2)
H1	0.3557	0.5125	0.5955	0.051*
N2	0.0986 (2)	0.35310 (5)	0.57304 (8)	0.0436 (2)
C1	0.2795 (2)	0.40708 (5)	0.52935 (9)	0.0412 (2)
C2	0.0662 (2)	0.45135 (6)	0.69742 (9)	0.0412 (2)
C3	−0.0238 (3)	0.49315 (7)	0.79538 (11)	0.0523 (3)
H3	0.0420	0.5416	0.8087	0.063*
C4	−0.2163 (3)	0.46000 (9)	0.87330 (12)	0.0623 (4)
H4	−0.2806	0.4868	0.9403	0.075*
C5	−0.3150 (3)	0.38814 (9)	0.85397 (12)	0.0625 (4)
H5	−0.4446	0.3677	0.9080	0.075*
C6	−0.2248 (3)	0.34587 (7)	0.75573 (11)	0.0543 (3)
H6	−0.2904	0.2974	0.7427	0.065*
C7	−0.0329 (2)	0.37902 (6)	0.67788 (9)	0.0421 (3)
C8	0.0605 (3)	0.27990 (6)	0.51808 (11)	0.0539 (3)
H8A	0.1497	0.2789	0.4385	0.065*
H8B	−0.1478	0.2697	0.5029	0.065*
C9	0.1941 (3)	0.22211 (6)	0.59936 (12)	0.0553 (3)
C10	0.2989 (4)	0.17785 (7)	0.66881 (15)	0.0737 (4)
H10	0.3795	0.1424	0.7281	0.088*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0709 (5)	0.0453 (4)	0.0429 (4)	−0.0091 (4)	0.0121 (4)	−0.0023 (3)
N1	0.0500 (5)	0.0341 (4)	0.0435 (5)	−0.0036 (3)	0.0030 (4)	0.0009 (3)
N2	0.0516 (5)	0.0355 (4)	0.0434 (5)	−0.0065 (4)	0.0002 (4)	0.0010 (3)
C1	0.0490 (6)	0.0359 (5)	0.0381 (5)	−0.0023 (4)	−0.0020 (4)	0.0038 (4)
C2	0.0389 (5)	0.0424 (5)	0.0415 (5)	0.0029 (4)	−0.0029 (4)	0.0030 (4)
C3	0.0491 (6)	0.0549 (7)	0.0525 (6)	0.0059 (5)	0.0004 (5)	−0.0075 (5)

C4	0.0502 (7)	0.0862 (10)	0.0506 (7)	0.0099 (6)	0.0061 (5)	−0.0070 (6)
C5	0.0464 (6)	0.0881 (10)	0.0536 (7)	−0.0025 (6)	0.0081 (5)	0.0120 (6)
C6	0.0478 (6)	0.0594 (7)	0.0555 (7)	−0.0086 (5)	0.0009 (5)	0.0114 (5)
C7	0.0401 (5)	0.0444 (6)	0.0411 (5)	−0.0010 (4)	−0.0038 (4)	0.0049 (4)
C8	0.0690 (8)	0.0412 (6)	0.0505 (6)	−0.0135 (5)	−0.0032 (5)	−0.0032 (5)
C9	0.0709 (8)	0.0365 (6)	0.0590 (7)	−0.0124 (5)	0.0083 (6)	−0.0038 (5)
C10	0.0977 (11)	0.0425 (7)	0.0799 (10)	−0.0040 (7)	−0.0020 (8)	0.0087 (6)

Geometric parameters (Å, º)

N1—C1	1.3583 (13)	C8—H8A	0.9700
N1—C2	1.3869 (13)	C8—H8B	0.9700
N1—H1	0.9458	C9—C10	1.1725 (19)
N2—C1	1.3760 (13)	C3—C4	1.3856 (18)
N2—C7	1.3900 (14)	C3—H3	0.9300
N2—C8	1.4500 (13)	C6—C5	1.3848 (19)
C2—C3	1.3775 (15)	C6—H6	0.9300
C2—C7	1.3894 (15)	C5—C4	1.381 (2)
O1—C1	1.2367 (13)	C5—H5	0.9300
C7—C6	1.3835 (15)	C4—H4	0.9300
C8—C9	1.4657 (17)	C10—H10	0.9580
C1—N1—C2	110.15 (9)	N2—C8—H8B	109.3
C1—N1—H1	124.5	C9—C8—H8B	109.3
C2—N1—H1	125.3	H8A—C8—H8B	108.0
C1—N2—C7	109.75 (9)	C10—C9—C8	177.04 (14)
C1—N2—C8	124.15 (9)	C2—C3—C4	117.20 (12)
C7—N2—C8	126.08 (9)	C2—C3—H3	121.4
C3—C2—N1	131.78 (10)	C4—C3—H3	121.4
C3—C2—C7	121.20 (10)	C7—C6—C5	116.98 (12)
N1—C2—C7	107.02 (9)	C7—C6—H6	121.5
C6—C7—C2	121.62 (10)	C5—C6—H6	121.5
C6—C7—N2	131.84 (10)	C4—C5—C6	121.32 (12)
C2—C7—N2	106.54 (9)	C4—C5—H5	119.3
O1—C1—N1	127.61 (9)	C6—C5—H5	119.3
O1—C1—N2	125.87 (9)	C5—C4—C3	121.67 (12)
N1—C1—N2	106.52 (9)	C5—C4—H4	119.2
N2—C8—C9	111.58 (9)	C3—C4—H4	119.2
N2—C8—H8A	109.3	C9—C10—H10	177.7
C9—C8—H8A	109.3		
C1—N1—C2—C3	178.95 (11)	C8—N2—C1—O1	−0.04 (17)
C1—N1—C2—C7	−0.44 (11)	C7—N2—C1—N1	−1.39 (11)
C3—C2—C7—C6	−0.13 (16)	C8—N2—C1—N1	−179.94 (9)
N1—C2—C7—C6	179.33 (9)	C1—N2—C8—C9	109.99 (12)
C3—C2—C7—N2	−179.88 (9)	C7—N2—C8—C9	−68.32 (15)
N1—C2—C7—N2	−0.42 (11)	N1—C2—C3—C4	−179.25 (10)
C1—N2—C7—C6	−178.59 (11)	C7—C2—C3—C4	0.07 (16)

C8—N2—C7—C6	−0.07 (18)	C2—C7—C6—C5	0.22 (16)
C1—N2—C7—C2	1.13 (11)	N2—C7—C6—C5	179.90 (11)
C8—N2—C7—C2	179.65 (10)	C7—C6—C5—C4	−0.25 (18)
C2—N1—C1—O1	−178.79 (10)	C6—C5—C4—C3	0.2 (2)
C2—N1—C1—N2	1.12 (11)	C2—C3—C4—C5	−0.10 (18)
C7—N2—C1—O1	178.52 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.95	1.88	2.8226 (12)	174
C10—H10···O1^{ii}	0.96	2.39	3.2541 (17)	149

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, −*y*+1/2, *z*+1/2.