Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Isopropenyl-1*H*-1,3-benzimidazol-2(3*H*)-one

Asmaa Saber,[a] Hafid Zouihri,[b] El Mokhtar Essassi[a] and Seik Weng Ng[c]*

[a]Laboratoire de Chimie Organique Hétérocyclique, Pôle de Compétences Pharmacochimie, Université Mohammed V-Agdal, BP 1014 Avenue Ibn Batout, Rabat, Morocco, [b]CNRST Division UATRS, Angle Allal Fassi/FAR, BP 8027 Hay Riad, Rabat, Morocco, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

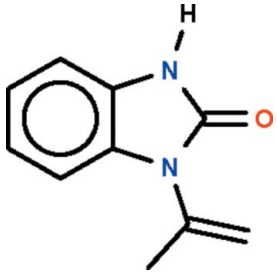
Received 27 April 2010; accepted 14 May 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.039; wR factor = 0.114; data-to-parameter ratio = 20.4.

In the title *N*-substituted benzimidazol-2-one, $C_{10}H_{10}N_2O$, the fused ring system is almost planar (r.m.s. deviation = 0.01 Å) and aligned at 57.9 (1)° with respect to the propenyl fragment. In the crystal, adjacent molecules are linked by pairs of N—H···O hydrogen bonds into inversion dimers.

Related literature

For the transformation of 1-isopropenyl-1,3-benzimidazol-2-one to other biologically-active compounds, see: Lakhrissi *et al.* (2010); Li *et al.* (2010). A shorter heating time in the synthesis leads to the formation of 4-methyl-2,3-dihydro-1*H*-1,5-benzodiazepin-2-one; see: Saber *et al.* (2010).



Experimental

Crystal data

$C_{10}H_{10}N_2O$ M_r = 174.20
Monoclinic, $C2/c$
a = 15.8724 (2) Å
b = 6.0971 (1) Å
c = 17.9313 (3) Å
β = 90.961 (2)°
V = 1735.07 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.35 × 0.30 × 0.18 mm

Data collection

Bruker X8 APEXII diffractometer
13930 measured reflections
2506 independent reflections
2231 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.114
S = 0.98
2506 reflections
123 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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}	0.87 (1)	1.95 (1)	2.811 (1)	172 (2)

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; 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).

We thank Université Mohammed V-Agdal and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2184).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Lakhrissi, B., Benksim, A., Massoui, M., Essassi, E. M., Lequart, V., Joly, N., Beaupeŕe, D., Wadouachi, A. & Martin, P. (2010). *Carbohydr. Res.* **343**, 421–433.
Li, S.-K., Ji, Z.-Q., Zhang, J.-W., Guo, Z.-Y. & Wu, W.-J. (2010). *J. Agric. Food Chem.* **58**, 2668–2672.
Saber, A., Zouihri, H., Essassi, E. M. & Ng, S. W. (2010). *Acta Cryst.* E**66**, o1408.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**. Submitted.

supporting information

Acta Cryst. (2010). E**66**, o1409 [https://doi.org/10.1107/S1600536810017897]

1-Isopropenyl-1*H*-1,3-benzimidazol-2(3*H*)-one

Asmaa Saber, Hafid Zouihri, El Mokhtar Essassi and Seik Weng Ng

S1. Comment

Benzimidazol-2-one derivatives possess a range of biological and pharmacological activities. Among the many compounds is *N*-isopropenyl benzimidazol-2-one, which can be further converted to 1-acyl-3-isopropenyl benzimidazol-2-ones that are active against *Botrytis cinerea* fungi that affect vegetables and fruits (Li *et al.* 2010). The reagent is also commercially available. We have recently reported the use of this reagent in the synthesis of some glucose-substituted benzimidazol-2-ones (Lakhrissi *et al.*, 2010). For the purpose of understanding the chemistry of these compounds, the crystal structure of the reagent is determined in the present study.

In the molecule of $C_{10}H_{10}N_2O$ (Scheme I, Fig. 1), the fused-ring is planar (r.m.s. deviation 0.01 Å); the propenyl fragment is aligned at 57.9 (1) ° with respect to the fused-ring. Adjacent molecules are linked about a center-of-inversion by an N–H···O hydrogen bond.

S2. Experimental

o-Phenylenediamine (1.0 g, 9 mmol) and ethyl acetoacetate (1.2 ml, 9 mmol) were heated in xylene (10 ml) for 6 hours. The mixture was set aside for the growth of colorless crystals of *N*-isopropenyl benzimidazol-2-one; yield 90%. When the heating time is shortened to 1 hour, the product is 4-methyl-2,3-dihydro-1*H*-1,5-benzodiazepin-2-one; details are given in another report (Saber *et al.*, 2010).

S3. Refinement

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

The amino H-atom was located in a difference Fourier map; the N–H distance was restrained to 0.86±0.01 Å. T; the temperature factor of the amino hydrogen atom was freely refined.

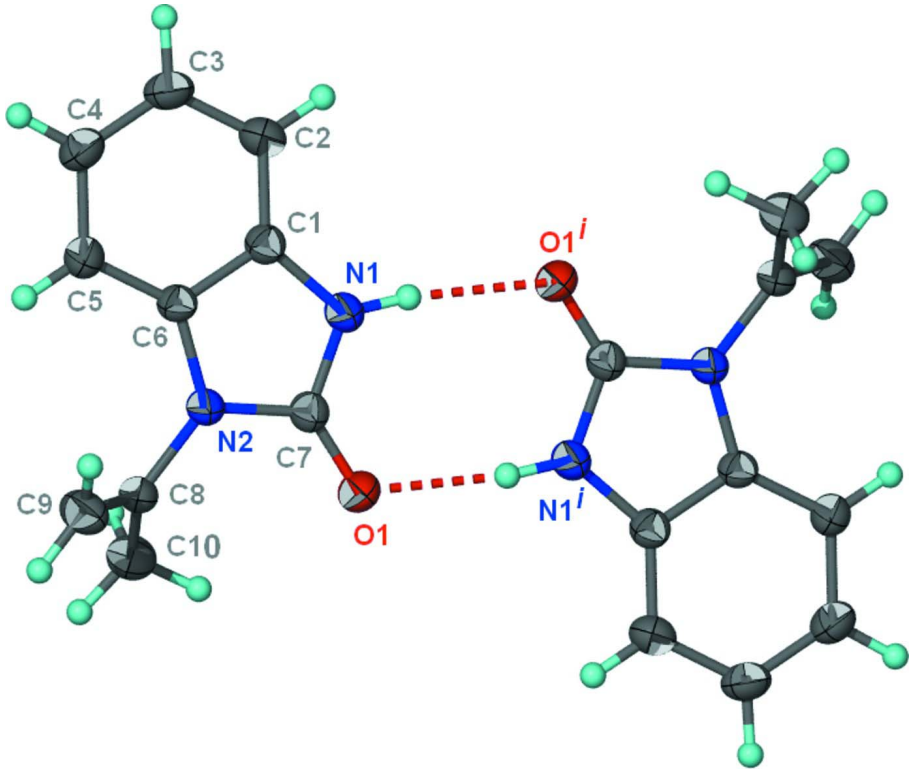


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the molecule of $C_{10}H_{10}N_2O$ at the 70% probability level shown as a hydrogen-bonded dimer; hydrogen atoms are drawn as spheres of arbitrary radius. Symmetry code: i = 1 - x, 1 - y, 1 - z.

1-Isopropenyl-1*H*-1,3-benzimidazol-2(3*H*)-one

Crystal data

$C_{10}H_{10}N_2O$
M_r = 174.20
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 15.8724 (2) Å
b = 6.0971 (1) Å
c = 17.9313 (3) Å
β = 90.961 (2)°
V = 1735.07 (5) Å^3
Z = 8
F(000) = 736
D_x = 1.334 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8296 reflections
θ = 2.3–35.0°
μ = 0.09 mm^{-1}
T = 100 K
Block, colorless
0.35 × 0.30 × 0.18 mm

Data collection

Bruker X8 APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
13930 measured reflections
2506 independent reflections
2231 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 30.0°, θ_{min} = 3.4°
h = −21→21
k = −8→8
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.114$
$S = 0.98$
2506 reflections
123 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0716P)^2 + 0.9009P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.58630 (4)	0.41270 (11)	0.43646 (4)	0.02815 (17)
N1	0.45280 (5)	0.26700 (13)	0.45678 (4)	0.02451 (18)
H1	0.4355 (10)	0.366 (2)	0.4880 (7)	0.048 (4)*
N2	0.53743 (5)	0.08911 (12)	0.38109 (4)	0.02211 (17)
C1	0.40921 (5)	0.08279 (14)	0.43226 (5)	0.02174 (18)
C2	0.32851 (6)	0.00950 (17)	0.44634 (5)	0.0275 (2)
H2	0.2922	0.0883	0.4783	0.033*
C3	0.30248 (6)	−0.18432 (17)	0.41176 (6)	0.0296 (2)
H3	0.2473	−0.2386	0.4201	0.036*
C4	0.35602 (6)	−0.29936 (17)	0.36524 (6)	0.0296 (2)
H4	0.3367	−0.4314	0.3426	0.035*
C5	0.43747 (6)	−0.22577 (15)	0.35092 (5)	0.0259 (2)
H5	0.4740	−0.3051	0.3193	0.031*
C6	0.46266 (5)	−0.03240 (14)	0.38485 (4)	0.02048 (18)
C7	0.53105 (6)	0.27304 (14)	0.42624 (5)	0.02226 (18)
C8	0.60775 (5)	0.04385 (15)	0.33453 (5)	0.02371 (19)
C9	0.64627 (6)	−0.14799 (17)	0.33983 (6)	0.0338 (2)
H9A	0.6272	−0.2545	0.3743	0.041*
H9B	0.6930	−0.1793	0.3091	0.041*
C10	0.62872 (7)	0.21916 (17)	0.27950 (6)	0.0327 (2)
H10A	0.6743	0.1682	0.2476	0.049*
H10B	0.6469	0.3517	0.3062	0.049*
H10C	0.5788	0.2524	0.2487	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0268 (3)	0.0240 (3)	0.0338 (4)	−0.0062 (2)	0.0053 (3)	−0.0065 (3)
N1	0.0231 (4)	0.0223 (4)	0.0284 (4)	−0.0013 (3)	0.0057 (3)	−0.0049 (3)
N2	0.0214 (4)	0.0209 (3)	0.0242 (3)	−0.0038 (3)	0.0054 (3)	−0.0036 (3)
C1	0.0218 (4)	0.0219 (4)	0.0216 (4)	−0.0003 (3)	0.0012 (3)	0.0005 (3)
C2	0.0215 (4)	0.0315 (5)	0.0298 (4)	−0.0009 (3)	0.0044 (3)	−0.0010 (3)
C3	0.0222 (4)	0.0350 (5)	0.0316 (5)	−0.0075 (3)	0.0017 (3)	0.0001 (4)

C4	0.0282 (5)	0.0304 (5)	0.0302 (4)	−0.0090 (4)	0.0004 (3)	−0.0036 (4)
C5	0.0265 (4)	0.0258 (4)	0.0255 (4)	−0.0044 (3)	0.0034 (3)	−0.0044 (3)
C6	0.0199 (4)	0.0216 (4)	0.0200 (4)	−0.0022 (3)	0.0016 (3)	0.0008 (3)
C7	0.0234 (4)	0.0204 (4)	0.0230 (4)	−0.0008 (3)	0.0027 (3)	−0.0013 (3)
C8	0.0215 (4)	0.0263 (4)	0.0235 (4)	−0.0056 (3)	0.0057 (3)	−0.0045 (3)
C9	0.0292 (5)	0.0292 (5)	0.0433 (6)	−0.0002 (4)	0.0114 (4)	−0.0055 (4)
C10	0.0352 (5)	0.0346 (5)	0.0287 (5)	−0.0088 (4)	0.0090 (4)	0.0014 (4)

Geometric parameters (Å, º)

O1—C7	1.2338 (11)	C3—H3	0.9500
N1—C7	1.3663 (11)	C4—C5	1.3963 (13)
N1—C1	1.3868 (11)	C4—H4	0.9500
N1—H1	0.871 (9)	C5—C6	1.3827 (12)
N2—C7	1.3878 (11)	C5—H5	0.9500
N2—C6	1.4016 (10)	C8—C9	1.3225 (14)
N2—C8	1.4319 (11)	C8—C10	1.4960 (13)
C1—C2	1.3839 (12)	C9—H9A	0.9500
C1—C6	1.3999 (11)	C9—H9B	0.9500
C2—C3	1.3939 (14)	C10—H10A	0.9800
C2—H2	0.9500	C10—H10B	0.9800
C3—C4	1.3907 (14)	C10—H10C	0.9800
C7—N1—C1	110.29 (7)	C4—C5—H5	121.5
C7—N1—H1	122.5 (11)	C5—C6—C1	121.42 (8)
C1—N1—H1	127.2 (11)	C5—C6—N2	131.94 (8)
C7—N2—C6	109.21 (7)	C1—C6—N2	106.63 (7)
C7—N2—C8	124.13 (7)	O1—C7—N1	127.42 (8)
C6—N2—C8	126.52 (7)	O1—C7—N2	125.86 (8)
C2—C1—N1	131.46 (8)	N1—C7—N2	106.72 (7)
C2—C1—C6	121.39 (8)	C9—C8—N2	119.50 (8)
N1—C1—C6	107.14 (7)	C9—C8—C10	124.87 (9)
C1—C2—C3	117.45 (9)	N2—C8—C10	115.54 (8)
C1—C2—H2	121.3	C8—C9—H9A	120.0
C3—C2—H2	121.3	C8—C9—H9B	120.0
C4—C3—C2	120.99 (9)	H9A—C9—H9B	120.0
C4—C3—H3	119.5	C8—C10—H10A	109.5
C2—C3—H3	119.5	C8—C10—H10B	109.5
C3—C4—C5	121.69 (9)	H10A—C10—H10B	109.5
C3—C4—H4	119.2	C8—C10—H10C	109.5
C5—C4—H4	119.2	H10A—C10—H10C	109.5
C6—C5—C4	117.05 (9)	H10B—C10—H10C	109.5
C6—C5—H5	121.5		
C7—N1—C1—C2	−178.46 (10)	C8—N2—C6—C5	4.24 (15)
C7—N1—C1—C6	0.49 (10)	C7—N2—C6—C1	1.11 (10)
N1—C1—C2—C3	179.14 (9)	C8—N2—C6—C1	−174.64 (8)
C6—C1—C2—C3	0.31 (14)	C1—N1—C7—O1	−179.45 (9)

C1—C2—C3—C4	0.29 (15)	C1—N1—C7—N2	0.19 (10)
C2—C3—C4—C5	−0.32 (16)	C6—N2—C7—O1	178.83 (9)
C3—C4—C5—C6	−0.25 (15)	C8—N2—C7—O1	−5.29 (15)
C4—C5—C6—C1	0.85 (13)	C6—N2—C7—N1	−0.81 (10)
C4—C5—C6—N2	−177.89 (9)	C8—N2—C7—N1	175.06 (8)
C2—C1—C6—C5	−0.91 (13)	C7—N2—C8—C9	127.09 (10)
N1—C1—C6—C5	−179.99 (8)	C6—N2—C8—C9	−57.76 (13)
C2—C1—C6—N2	178.11 (8)	C7—N2—C8—C10	−56.22 (12)
N1—C1—C6—N2	−0.97 (9)	C6—N2—C8—C10	118.93 (9)
C7—N2—C6—C5	179.99 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.87 (1)	1.95 (1)	2.811 (1)	172 (2)

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