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5-(4-Hydroxyphenyl)imidazolidine-2,4-dione

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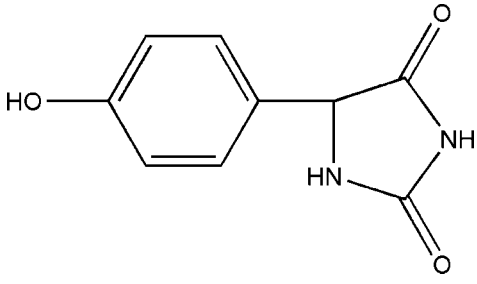
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 11.4.

The title compound, $C_9H_8N_2O_3$, was prepared by reaction of phenol, glyoxylic acid and urea in water. The imidazolidine ring adopts an almost planar conformation (r.m.s. deviation = 0.012 Å) and is twisted by 89.3 (1)° relative to the benzene ring. In the crystal, molecules are linked by N—H···O and O—H···O hydrogen bonds into a three-dimensional framework.

Related literature

For general background to the synthesis and applications of hydantoin derivatives, see: Liu & Zhao (2001); Dhar *et al.* (2002); Goodnow & Kang (2003). For related compounds, see: Ji *et al.* (2002).



Experimental

Crystal data

$C_9H_8N_2O_3$ M_r = 192.17
Monoclinic, $P2_1/c$
a = 10.3694 (11) Å
b = 6.9914 (8) Å
c = 12.3857 (13) Å
β = 105.619 (2)°
V = 864.76 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
4721 measured reflections
1558 independent reflections
1100 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 1.02
1558 reflections
137 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O4^{i}	0.883 (18)	1.952 (19)	2.8180 (19)	166.7 (17)
N1—H1···O4^{ii}	0.85 (2)	2.535 (19)	3.204 (2)	136.5 (16)
N1—H1···O6^{iii}	0.85 (2)	2.36 (2)	3.067 (2)	141.1 (17)
O6—H6···O5^{iv}	0.95 (2)	1.78 (2)	2.7223 (18)	169.0 (18)

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x, -y, -z+1$; (iv) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: KQ2013).

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supporting information

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S1. Comment

Hydantoin derivatives can be used as intermediates in pharmaceutical products, pesticides and photosensitive material. It is very important to the development of hydantoins compounds. Pharmacological functions of hydantoin derivatives are mainly shown in antibacterial (Liu & Zhao, 2001), diminishing inflammation (Dhar *et al.*, 2002), relieving cough and asthma, lowering blood sugar (Goodnow & Kang, 2003), and inhibiting agent of uremic toxin. Different substituted hydantoin and its derivatives show good application future, such as the treatment of diabetes, kidney disease, autoimmune disease and blood disease. The spectrum of hydantoin derivatives is broad as bacterial disinfectant. They are widely used in aquaculture, pest and disease control, disinfection treatment of health equipment, mildew prevention and control of crops, preservation of vegetable & Fruit, and mildew anti-corrosion of industrial products and living goods.

In the molecule of the title compound, $C_9H_8N_2O_3$, **I** (Fig. 1) bond lengths and angles are generally normal (Ji *et al.*, 2002). The imidazolidine ring adopts a planar conformation (r.m.s. deviation is 0.012 Å) and is twisted by 89.3 (1)° relative to the benzene plane.

In the crystal, molecules are bound by intermolecular N—H···O and O—H···O hydrogen bonds (Table 1) into three-dimensional framework (Fig. 2).

S2. Experimental

The title compound was prepared by reaction of phenol (0.05 mol), glyoxylic acid (0.06 mol) and urea (0.06 mol) in hydrochloric acid (37%, 80 ml) at 370 K for 6 h, cooling, filtering, affording the tile compound by recrystallization in water. Single crystals of the title compound suitable for X-ray measurements was obtained by recrystallization from ethanol at room temperature.

S3. Refinement

The hydroxyl and amino hydrogen atoms were objectively localized in the difference-Fourier map and refined isotropically with fixed displacement parameters. The other hydrogen atoms were placed in the calculated positions with C—H distances = 0.93–0.98 Å and refined in the riding model with fixed isotropic displacement parameters: U_{iso}(H) = 1.2U_{eq}(C).

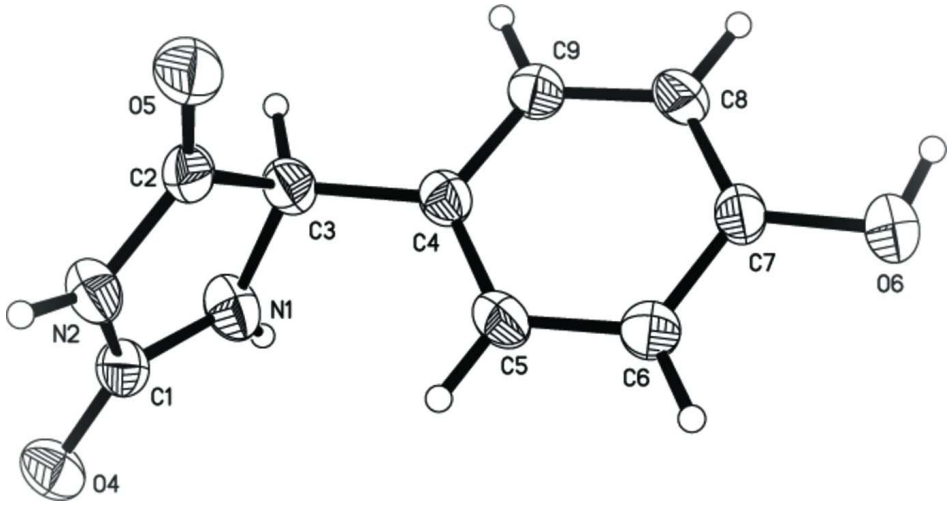

Figure 1

Molecular structure of **I**. Displacement ellipsoids are presented at the 40% probability level. H atoms are depicted as small spheres of arbitrary radius.

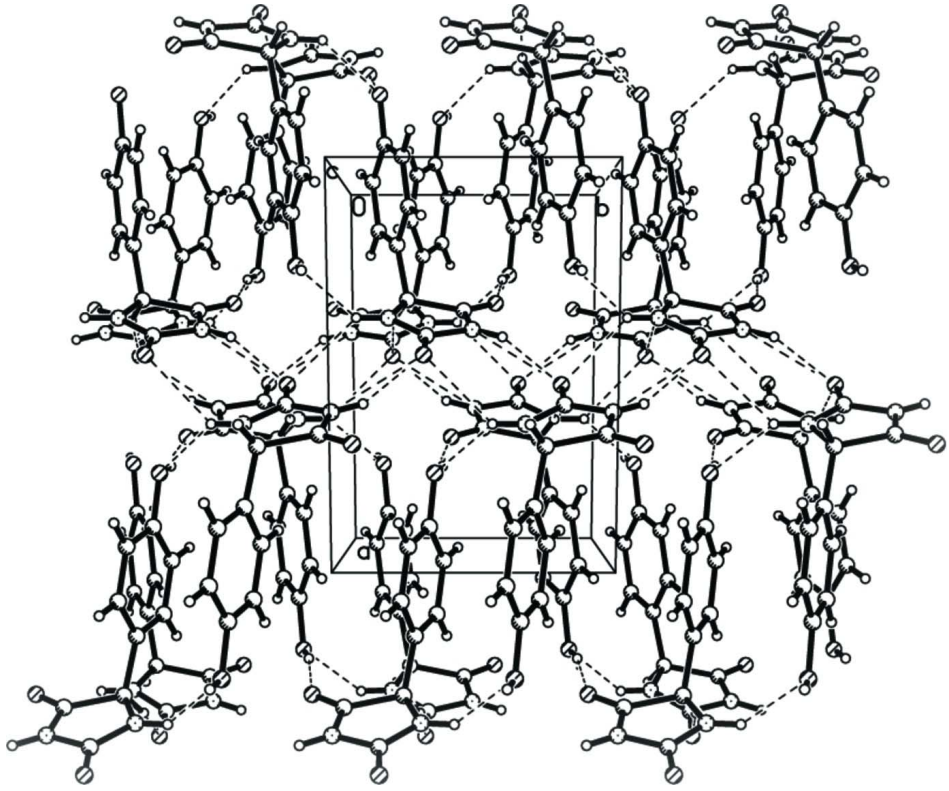

Figure 2

A portion of the crystal structure of **I** viewed along [001]. The intermolecular hydrogen bonding interactions are depicted by dashed lines.

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Crystal data

$C_9H_8N_2O_3$
M_r = 192.17
Monoclinic, $P2_1/c$
a = 10.3694 (11) Å
b = 6.9914 (8) Å
c = 12.3857 (13) Å
β = 105.619 (2)°
V = 864.76 (16) Å^3
Z = 4
$F(000)$ = 400
D_x = 1.476 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 933 reflections
θ = 2.0–25.0°
μ = 0.11 mm^{-1}
T = 296 K
Rectangle, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
4721 measured reflections
1558 independent reflections
1100 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.2°, θ_{min} = 2.0°
h = −12→12
k = −8→8
l = −7→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 1.02
1558 reflections
137 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.0206P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: *SHELXL2013* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.024 (3)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.36582 (16)	0.1852 (2)	0.60788 (13)	0.0438 (4)
H1	0.3651 (18)	0.070 (3)	0.6298 (15)	0.053*
N2	0.39496 (14)	0.4952 (2)	0.61795 (12)	0.0394 (4)
H2	0.4272 (18)	0.605 (3)	0.6494 (15)	0.047*
O4	0.46179 (12)	0.32043 (18)	0.78108 (10)	0.0464 (4)
O5	0.32237 (12)	0.58433 (19)	0.43383 (10)	0.0508 (4)
O6	−0.23743 (12)	0.1408 (2)	0.29172 (11)	0.0512 (4)
H6	−0.2595 (19)	0.108 (3)	0.2145 (17)	0.061*

C1	0.41256 (16)	0.3268 (3)	0.67946 (15)	0.0360 (4)
C2	0.34366 (16)	0.4631 (3)	0.50733 (15)	0.0362 (4)
C3	0.31532 (17)	0.2501 (2)	0.49270 (14)	0.0385 (5)
H3	0.3691	0.1943	0.4466	0.046*
C4	0.16868 (17)	0.2098 (2)	0.43983 (14)	0.0353 (4)
C5	0.07338 (17)	0.2567 (3)	0.49525 (15)	0.0410 (5)
H5	0.1009	0.3060	0.5676	0.049*
C6	−0.06081 (18)	0.2319 (3)	0.44558 (15)	0.0417 (5)
H6A	−0.1233	0.2633	0.4842	0.050*
C7	−0.10245 (17)	0.1601 (2)	0.33802 (14)	0.0366 (4)
C8	−0.00956 (17)	0.1091 (3)	0.28186 (14)	0.0413 (5)
H8	−0.0374	0.0583	0.2099	0.050*
C9	0.12569 (18)	0.1341 (3)	0.33336 (14)	0.0414 (5)
H9	0.1883	0.0992	0.2955	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0489 (10)	0.0338 (9)	0.0412 (10)	−0.0001 (8)	−0.0011 (7)	0.0047 (7)
N2	0.0423 (9)	0.0360 (9)	0.0336 (9)	−0.0046 (7)	−0.0009 (7)	0.0005 (7)
O4	0.0472 (8)	0.0544 (9)	0.0312 (8)	0.0075 (6)	−0.0002 (6)	0.0051 (6)
O5	0.0534 (9)	0.0547 (9)	0.0394 (8)	−0.0061 (7)	0.0038 (6)	0.0111 (7)
O6	0.0360 (8)	0.0701 (10)	0.0427 (8)	−0.0081 (6)	0.0023 (6)	−0.0054 (7)
C1	0.0277 (9)	0.0427 (11)	0.0348 (11)	0.0036 (8)	0.0035 (8)	0.0016 (8)
C2	0.0281 (9)	0.0437 (11)	0.0340 (11)	−0.0025 (8)	0.0036 (8)	0.0027 (9)
C3	0.0357 (10)	0.0431 (11)	0.0342 (10)	0.0011 (8)	0.0054 (8)	−0.0028 (8)
C4	0.0374 (10)	0.0326 (10)	0.0338 (10)	−0.0025 (8)	0.0063 (8)	−0.0021 (8)
C5	0.0433 (12)	0.0468 (11)	0.0310 (10)	−0.0035 (9)	0.0068 (8)	−0.0100 (8)
C6	0.0394 (11)	0.0483 (12)	0.0385 (11)	−0.0017 (9)	0.0126 (8)	−0.0076 (9)
C7	0.0330 (10)	0.0377 (11)	0.0359 (10)	−0.0036 (8)	0.0040 (8)	0.0007 (8)
C8	0.0460 (11)	0.0463 (11)	0.0297 (10)	−0.0078 (9)	0.0071 (8)	−0.0090 (8)
C9	0.0399 (11)	0.0489 (12)	0.0368 (11)	−0.0028 (9)	0.0124 (8)	−0.0078 (9)

Geometric parameters (Å, º)

N1—C1	1.330 (2)	C3—H3	0.9800
N1—C3	1.454 (2)	C4—C9	1.379 (2)
N1—H1	0.85 (2)	C4—C5	1.386 (3)
N2—C2	1.348 (2)	C5—C6	1.373 (2)
N2—C1	1.387 (2)	C5—H5	0.9300
N2—H2	0.883 (18)	C6—C7	1.380 (2)
O4—C1	1.2251 (18)	C6—H6A	0.9300
O5—C2	1.220 (2)	C7—C8	1.378 (3)
O6—C7	1.3690 (19)	C8—C9	1.387 (2)
O6—H6	0.95 (2)	C8—H8	0.9300
C2—C3	1.519 (2)	C9—H9	0.9300
C3—C4	1.511 (2)		

C1—N1—C3	113.08 (15)	C9—C4—C5	118.33 (16)
C1—N1—H1	121.6 (13)	C9—C4—C3	120.95 (17)
C3—N1—H1	125.3 (13)	C5—C4—C3	120.65 (16)
C2—N2—C1	111.98 (15)	C6—C5—C4	121.34 (17)
C2—N2—H2	126.3 (12)	C6—C5—H5	119.3
C1—N2—H2	121.0 (12)	C4—C5—H5	119.3
C7—O6—H6	112.8 (12)	C5—C6—C7	119.65 (17)
O4—C1—N1	129.33 (17)	C5—C6—H6A	120.2
O4—C1—N2	123.50 (17)	C7—C6—H6A	120.2
N1—C1—N2	107.17 (15)	O6—C7—C8	122.53 (16)
O5—C2—N2	125.82 (17)	O6—C7—C6	117.33 (16)
O5—C2—C3	127.01 (16)	C8—C7—C6	120.13 (15)
N2—C2—C3	107.16 (15)	C7—C8—C9	119.54 (16)
N1—C3—C4	114.94 (15)	C7—C8—H8	120.2
N1—C3—C2	100.48 (13)	C9—C8—H8	120.2
C4—C3—C2	111.97 (14)	C4—C9—C8	120.98 (17)
N1—C3—H3	109.7	C4—C9—H9	119.5
C4—C3—H3	109.7	C8—C9—H9	119.5
C2—C3—H3	109.7		

C3—N1—C1—O4	−179.77 (17)	C2—C3—C4—C9	112.19 (19)
C3—N1—C1—N2	0.8 (2)	N1—C3—C4—C5	49.1 (2)
C2—N2—C1—O4	177.58 (16)	C2—C3—C4—C5	−64.7 (2)
C2—N2—C1—N1	−3.0 (2)	C9—C4—C5—C6	−1.0 (3)
C1—N2—C2—O5	−177.36 (17)	C3—C4—C5—C6	175.96 (17)
C1—N2—C2—C3	3.78 (19)	C4—C5—C6—C7	−0.5 (3)
C1—N1—C3—C4	−119.10 (17)	C5—C6—C7—O6	−179.04 (16)
C1—N1—C3—C2	1.27 (19)	C5—C6—C7—C8	1.6 (3)
O5—C2—C3—N1	178.20 (17)	O6—C7—C8—C9	179.43 (16)
N2—C2—C3—N1	−2.96 (17)	C6—C7—C8—C9	−1.3 (3)
O5—C2—C3—C4	−59.3 (2)	C5—C4—C9—C8	1.4 (3)
N2—C2—C3—C4	119.51 (16)	C3—C4—C9—C8	−175.60 (17)
N1—C3—C4—C9	−133.99 (17)	C7—C8—C9—C4	−0.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4^{i}	0.883 (18)	1.952 (19)	2.8180 (19)	166.7 (17)
N1—H1···O4^{ii}	0.85 (2)	2.535 (19)	3.204 (2)	136.5 (16)
N1—H1···O6^{iii}	0.85 (2)	2.36 (2)	3.067 (2)	141.1 (17)
O6—H6···O5^{iv}	0.95 (2)	1.78 (2)	2.7223 (18)	169.0 (18)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) −*x*+1, *y*−1/2, −*z*+3/2; (iii) −*x*, −*y*, −*z*+1; (iv) −*x*, *y*−1/2, −*z*+1/2.