# 3-Hydroxymethyl-1-(4-methoxyphenyl)-imidazolidine-2,4-dione

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In the title molecule, $C_{11}H_{12}N_2O_4$, the dihedral angle between the benzene ring and imidazolidine ring is 7.1 (5)°. In the crystal structure, the hydroxy groups are involved in the formation of intermolecular O—H⋯O hydrogen bonds, which link the molecules related by translation into $C(2)$ chains along the $b$ axis.

## Related literature

For related structures, see: Gerdil (1960); Sun *et al.* (2010). For details of the synthesis, see: Niwata *et al.* (1997).
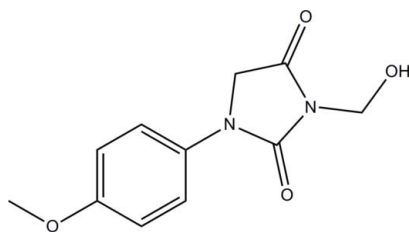


## Experimental

*Crystal data*

$C_{11}H_{12}N_2O_4$
$M_r = 236.23$
Monoclinic, $P2_1/c$
$a = 21.280$ (4) Å
$b = 6.3309$ (13) Å
$c = 7.8813$ (16) Å
$\beta = 100.52$ (3)°
$V = 1043.9$ (4) Å$^3$
$Z = 4$
Mo $K\alpha$ radiation

$\mu = 0.12$ mm$^{-1}$
$T = 113$ K
$0.20 \times 0.18 \times 0.12$ mm

*Data collection*

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.977$, $T_{max} = 0.986$

7503 measured reflections
1841 independent reflections
1540 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.112$
$S = 1.09$
1841 reflections

156 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.18$ e Å$^{-3}$
$\Delta\rho_{min} = -0.23$ e Å$^{-3}$

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| O3—H3⋯O4$^i$ | 0.82 | 1.92 | 2.7346 (17) | 174 |

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

## References

Gerdil, R. (1960). *Acta Cryst.* **13**, 165–166.

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sun, S.-X., Zhang, H., Cheng, X.-C., Wang, R.-L. & Dong, W.-L. (2010). *Acta Cryst.* E**66**, o1308.

**supplementary materials**

### 3-Hydroxymethyl-1-(4-methoxyphenyl)imidazolidine-2,4-dione

**X.-C. Cheng, J.-J. Hou, R.-L. Wang and W.-L. Dong**

#### Comment

During the research of novel antidiabetic agents, we found that imidazolidine-2,4-dione derivatives had potent antidiabetic activities. The crystal structure of the title compound was determined to investigate the relationship between structure and antidiabetic activity.

In the title compound, all bond lengths and angles are normal and in a good agreement with those reported previously (Gerdil, 1960; Sun *et al.*, 2010). The dihedral angle between the benzene ring (C2—C7) and imidazolidine ring (C9—C10/N1/N2) is 7.1 (5)°. In the crystal structure, the hydroxy groups are involved in formaton of intermolecular O—H⋯O hydrogen bonds (Table 1), which link the molecules related by translation along axis *b* into linear chains.

#### Experimental

A mixture of 1-(4-methoxyphenyl)imidazolidine-2,4-dione (0.27 g, 1.32 mmol), 37% formaldehyde (2.1 ml, 27.9 mmol), and methanol (8 ml) was stirred at 70 ° C for 2 h. After the reaction, water (8 ml) was added and the precipitate was filtered and washed with water to give 3-(hydroxymethyl)-1-(4-methoxyphenyl)imidazolidine-2,4-dione (0.27 g, 90% yield) (Niwata *et al.*, 1997). Crystals suitable for X-ray diffraction were obtained through slow evaporation of a solution of the pure title compound in dichloromethane/methanol (1/1 by volume).

#### Refinement

All H atoms were found on difference maps, with C—H = 0.95–0.99 Å and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ for aryl and methylene H atoms and $1.5U_{eq}(C,O)$ for the methyl and hydroxy H atoms.
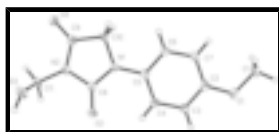
#### Figures



Fig. 1. View of the title compound, with displacement ellipsoids drawn at the 40% probability level.

### 3-Hydroxymethyl-1-(4-methoxyphenyl)imidazolidine-2,4-dione

*Crystal data*

| | |
|---|---|
| $C_{11}H_{12}N_2O_4$ | $F(000) = 496$ |
| $M_r = 236.23$ | $D_x = 1.503$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |

# supplementary materials

Hall symbol: -P 2ybc

$a = 21.280$ (4) Å

$b = 6.3309$ (13) Å

$c = 7.8813$ (16) Å

$\beta = 100.52$ (3)°

$V = 1043.9$ (4) Å$^3$

$Z = 4$

Cell parameters from 2988 reflections

$\theta = 2.0–27.9°$

$\mu = 0.12$ mm$^{-1}$

$T = 113$ K

Platelet, colorless

$0.20 \times 0.18 \times 0.12$ mm

*Data collection*

| | |
|---|---|
| Rigaku Saturn CCD area-detector diffractometer | 1841 independent reflections |
| Radiation source: rotating anode | 1540 reflections with $I > 2\sigma(I)$ |
| confocal | $R_{int} = 0.042$ |
| Detector resolution: 7.31 pixels mm$^{-1}$ | $\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$ |
| $\omega$ and $\varphi$ scans | $h = -25 \rightarrow 23$ |
| Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005) | $k = -7 \rightarrow 7$ |
| $T_{min} = 0.977$, $T_{max} = 0.986$ | $l = -7 \rightarrow 9$ |
| 7503 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.112$ | H-atom parameters constrained |
| $S = 1.09$ | $w = 1/[\sigma^2(F_o^2) + (0.0696P)^2 + 0.0281P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 1841 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 156 parameters | $\Delta\rho_{max} = 0.18$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.23$ e Å$^{-3}$ |

*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.

**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 | 0.06206 (5) | 0.43299 (18) | 0.14946 (13) | 0.0262 (3) |
| O2 | 0.31479 (5) | 0.92240 (17) | 0.56402 (13) | 0.0239 (3) |
| O3 | 0.41891 (6) | 0.98695 (18) | 0.93286 (14) | 0.0310 (3) |
| H3 | 0.4247 | 1.1116 | 0.9119 | 0.046* |
| O4 | 0.43355 (5) | 0.41010 (18) | 0.88227 (13) | 0.0263 (3) |
| N1 | 0.29378 (6) | 0.5666 (2) | 0.60155 (15) | 0.0189 (3) |
| N2 | 0.38408 (6) | 0.7058 (2) | 0.74760 (15) | 0.0198 (3) |
| C1 | 0.02888 (8) | 0.2377 (3) | 0.1525 (2) | 0.0333 (4) |
| H1A | 0.0536 | 0.1259 | 0.1151 | 0.050* |
| H1B | −0.0118 | 0.2463 | 0.0767 | 0.050* |
| H1C | 0.0225 | 0.2095 | 0.2679 | 0.050* |
| C2 | 0.11895 (7) | 0.4547 (3) | 0.26381 (19) | 0.0207 (4) |
| C3 | 0.14827 (7) | 0.6511 (3) | 0.26585 (19) | 0.0229 (4) |
| H3A | 0.1292 | 0.7568 | 0.1921 | 0.027* |
| C4 | 0.20547 (7) | 0.6918 (3) | 0.37598 (19) | 0.0216 (4) |
| H4 | 0.2243 | 0.8244 | 0.3768 | 0.026* |
| C5 | 0.23490 (7) | 0.5332 (3) | 0.48603 (18) | 0.0188 (4) |
| C6 | 0.20577 (7) | 0.3369 (3) | 0.48223 (18) | 0.0208 (4) |
| H6 | 0.2252 | 0.2302 | 0.5544 | 0.025* |
| C7 | 0.14802 (7) | 0.2966 (3) | 0.3726 (2) | 0.0234 (4) |
| H7 | 0.1290 | 0.1644 | 0.3722 | 0.028* |
| C8 | 0.32780 (7) | 0.7496 (2) | 0.62781 (19) | 0.0188 (4) |
| C9 | 0.38857 (7) | 0.4969 (3) | 0.78904 (18) | 0.0208 (4) |
| C10 | 0.32821 (7) | 0.3927 (3) | 0.69862 (18) | 0.0208 (4) |
| H10A | 0.3374 | 0.2813 | 0.6222 | 0.025* |
| H10B | 0.3041 | 0.3342 | 0.7807 | 0.025* |
| C11 | 0.43450 (7) | 0.8604 (3) | 0.79990 (19) | 0.0237 (4) |
| H11A | 0.4748 | 0.7887 | 0.8400 | 0.028* |
| H11B | 0.4392 | 0.9482 | 0.7021 | 0.028* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0191 (6) | 0.0278 (7) | 0.0292 (6) | −0.0026 (5) | −0.0022 (5) | −0.0004 (5) |
| O2 | 0.0255 (6) | 0.0176 (6) | 0.0282 (6) | −0.0021 (5) | 0.0038 (5) | 0.0026 (5) |
| O3 | 0.0468 (8) | 0.0223 (7) | 0.0258 (6) | −0.0109 (6) | 0.0117 (5) | −0.0066 (5) |
| O4 | 0.0242 (6) | 0.0259 (7) | 0.0264 (6) | 0.0028 (5) | −0.0021 (5) | −0.0016 (5) |
| N1 | 0.0182 (7) | 0.0165 (7) | 0.0207 (7) | −0.0004 (5) | 0.0000 (5) | 0.0008 (5) |
| N2 | 0.0198 (7) | 0.0196 (7) | 0.0196 (7) | −0.0036 (5) | 0.0026 (5) | −0.0025 (5) |
| C1 | 0.0251 (9) | 0.0371 (11) | 0.0347 (9) | −0.0111 (8) | −0.0024 (7) | 0.0010 (8) |
| C2 | 0.0170 (8) | 0.0262 (9) | 0.0189 (8) | 0.0003 (6) | 0.0029 (6) | −0.0035 (7) |
| C3 | 0.0215 (8) | 0.0233 (9) | 0.0234 (8) | 0.0019 (7) | 0.0028 (6) | 0.0033 (7) |
| C4 | 0.0213 (8) | 0.0189 (8) | 0.0247 (8) | −0.0008 (6) | 0.0046 (6) | 0.0014 (7) |
| C5 | 0.0180 (8) | 0.0214 (8) | 0.0175 (8) | −0.0004 (6) | 0.0048 (6) | −0.0021 (6) |

| | | | | | |
|---|---|---|---|---|---|
| C6 | 0.0207 (8) | 0.0195 (9) | 0.0216 (8) | 0.0005 (6) | 0.0024 (6) | 0.0019 (6) |
| C7 | 0.0231 (8) | 0.0208 (9) | 0.0262 (8) | −0.0049 (7) | 0.0040 (6) | −0.0017 (7) |
| C8 | 0.0188 (8) | 0.0205 (8) | 0.0182 (8) | −0.0021 (6) | 0.0063 (6) | −0.0023 (6) |
| C9 | 0.0224 (8) | 0.0222 (9) | 0.0182 (8) | 0.0012 (7) | 0.0049 (6) | −0.0027 (6) |
| C10 | 0.0222 (8) | 0.0181 (8) | 0.0211 (8) | 0.0004 (6) | 0.0017 (6) | −0.0001 (6) |
| C11 | 0.0206 (8) | 0.0267 (9) | 0.0235 (8) | −0.0069 (7) | 0.0032 (6) | −0.0034 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C2 | 1.3778 (18) | C2—C7 | 1.388 (2) |
| O1—C1 | 1.426 (2) | C2—C3 | 1.390 (2) |
| O2—C8 | 1.2147 (19) | C3—C4 | 1.384 (2) |
| O3—C11 | 1.406 (2) | C3—H3A | 0.9300 |
| O3—H3 | 0.8200 | C4—C5 | 1.398 (2) |
| O4—C9 | 1.2252 (19) | C4—H4 | 0.9300 |
| N1—C8 | 1.3614 (19) | C5—C6 | 1.387 (2) |
| N1—C5 | 1.4238 (19) | C6—C7 | 1.391 (2) |
| N1—C10 | 1.460 (2) | C6—H6 | 0.9300 |
| N2—C9 | 1.361 (2) | C7—H7 | 0.9300 |
| N2—C8 | 1.411 (2) | C9—C10 | 1.503 (2) |
| N2—C11 | 1.4556 (19) | C10—H10A | 0.9700 |
| C1—H1A | 0.9600 | C10—H10B | 0.9700 |
| C1—H1B | 0.9600 | C11—H11A | 0.9700 |
| C1—H1C | 0.9600 | C11—H11B | 0.9700 |
| | | | |
| C2—O1—C1 | 117.01 (13) | C4—C5—N1 | 122.16 (14) |
| C11—O3—H3 | 109.5 | C5—C6—C7 | 121.23 (15) |
| C8—N1—C5 | 127.24 (13) | C5—C6—H6 | 119.4 |
| C8—N1—C10 | 111.11 (12) | C7—C6—H6 | 119.4 |
| C5—N1—C10 | 121.46 (13) | C2—C7—C6 | 119.68 (15) |
| C9—N2—C8 | 111.44 (12) | C2—C7—H7 | 120.2 |
| C9—N2—C11 | 124.73 (13) | C6—C7—H7 | 120.2 |
| C8—N2—C11 | 123.31 (13) | O2—C8—N1 | 128.95 (14) |
| O1—C1—H1A | 109.5 | O2—C8—N2 | 123.76 (14) |
| O1—C1—H1B | 109.5 | N1—C8—N2 | 107.30 (13) |
| H1A—C1—H1B | 109.5 | O4—C9—N2 | 126.35 (15) |
| O1—C1—H1C | 109.5 | O4—C9—C10 | 126.42 (16) |
| H1A—C1—H1C | 109.5 | N2—C9—C10 | 107.23 (12) |
| H1B—C1—H1C | 109.5 | N1—C10—C9 | 102.77 (13) |
| O1—C2—C7 | 124.84 (15) | N1—C10—H10A | 111.2 |
| O1—C2—C3 | 115.85 (14) | C9—C10—H10A | 111.2 |
| C7—C2—C3 | 119.31 (15) | N1—C10—H10B | 111.2 |
| C4—C3—C2 | 121.01 (15) | C9—C10—H10B | 111.2 |
| C4—C3—H3A | 119.5 | H10A—C10—H10B | 109.1 |
| C2—C3—H3A | 119.5 | O3—C11—N2 | 109.40 (12) |
| C3—C4—C5 | 119.91 (15) | O3—C11—H11A | 109.8 |
| C3—C4—H4 | 120.0 | N2—C11—H11A | 109.8 |
| C5—C4—H4 | 120.0 | O3—C11—H11B | 109.8 |
| C6—C5—C4 | 118.84 (14) | N2—C11—H11B | 109.8 |
| C6—C5—N1 | 119.00 (14) | H11A—C11—H11B | 108.2 |

| | | | |
|---|---|---|---|
| C1—O1—C2—C7 | 4.5 (2) | C10—N1—C8—O2 | 177.46 (15) |
| C1—O1—C2—C3 | −176.06 (14) | C5—N1—C8—N2 | −177.40 (13) |
| O1—C2—C3—C4 | 179.71 (13) | C10—N1—C8—N2 | −2.44 (17) |
| C7—C2—C3—C4 | −0.8 (2) | C9—N2—C8—O2 | −175.85 (14) |
| C2—C3—C4—C5 | 0.7 (2) | C11—N2—C8—O2 | −3.8 (2) |
| C3—C4—C5—C6 | 0.0 (2) | C9—N2—C8—N1 | 4.06 (17) |
| C3—C4—C5—N1 | 179.89 (14) | C11—N2—C8—N1 | 176.11 (12) |
| C8—N1—C5—C6 | −177.26 (14) | C8—N2—C9—O4 | 175.87 (14) |
| C10—N1—C5—C6 | 8.2 (2) | C11—N2—C9—O4 | 4.0 (2) |
| C8—N1—C5—C4 | 2.8 (2) | C8—N2—C9—C10 | −3.93 (17) |
| C10—N1—C5—C4 | −171.66 (14) | C11—N2—C9—C10 | −175.84 (12) |
| C4—C5—C6—C7 | −0.5 (2) | C8—N1—C10—C9 | 0.15 (15) |
| N1—C5—C6—C7 | 179.56 (14) | C5—N1—C10—C9 | 175.45 (13) |
| O1—C2—C7—C6 | 179.69 (13) | O4—C9—C10—N1 | −177.52 (15) |
| C3—C2—C7—C6 | 0.2 (2) | N2—C9—C10—N1 | 2.27 (15) |
| C5—C6—C7—C2 | 0.4 (2) | C9—N2—C11—O3 | −105.04 (16) |
| C5—N1—C8—O2 | 2.5 (3) | C8—N2—C11—O3 | 83.98 (17) |

*Hydrogen-bond geometry (Å, °)*

| D—H⋯A | D—H | H⋯A | D⋯A | D—H⋯A |
|---|---|---|---|---|
| O3—H3⋯O4[i] | 0.82 | 1.92 | 2.7346 (17) | 174. |

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

**Fig. 1**