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1-(4-Methoxyphenyl)imidazolidine-2,4-dione

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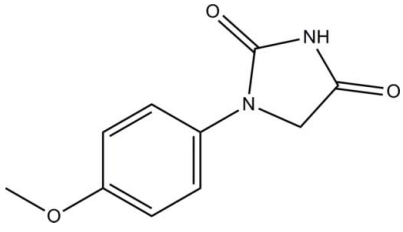
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.064; wR factor = 0.151; data-to-parameter ratio = 15.5.

In the title compound, $C_{10}H_{10}N_2O_3$, the dihedral angle between the benzene and imidazolidine rings is 6.0 (4)°, consistent with an essentially planar molecule. In the crystal, intermolecular N—H···O hydrogen bonding between centrosymmetrically related molecules leads to loosely associated dimeric aggregates. These are connected into a three-dimensional network by C—H···O interactions, as well as π–π interactions [centroid–centroid distances = 3.705 (3) and 3.622 (3) Å] between the imidazolidine and benzene rings.

Related literature

For related structures, see: Gerdil (1960). For the synthesis, see: Niwata *et al.* (1997); Kurzer *et al.* (1963).



Experimental

Crystal data

$C_{10}H_{10}N_2O_3$
M_r = 206.20
Monoclinic, $P2_1/c$
a = 4.9993 (10) Å
b = 6.1566 (12) Å
c = 30.052 (6) Å
β = 93.91 (3)°
V = 922.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 113 K
0.24 × 0.12 × 0.10 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.974, T_{max} = 0.989
6955 measured reflections
2203 independent reflections
1507 reflections with $I > 2\sigma(I)$
R_{int} = 0.078

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.151
S = 1.05
2203 reflections
142 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 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}	0.91 (1)	1.95 (1)	2.8512 (19)	172 (2)
C2—H2A···O2^{ii}	0.99	2.34	3.291 (2)	160
C8—H8···O2^{iii}	0.95	2.42	3.203 (2)	140

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $x, y+1, z$; (iii) $x+1, y+1, z$.

Data collection: *CrystalClear* (Rigaku/MSC, 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2669).

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supporting information

Acta Cryst. (2010). E**66**, o1308 [https://doi.org/10.1107/S1600536810016478]

1-(4-Methoxyphenyl)imidazolidine-2,4-dione

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S1. Comment

During an investigation of new anti-diabetic drugs, we found that imidazolidinediones (IZD's) have good anti-diabetic activities. The crystal structure determination of the title compound, (I), was undertaken to investigate the relationship between structure and anti-diabetic activity.

In title compound, $C_{10}H_{10}N_2O_3$, bond lengths and angles are normal and in a good agreement with those reported previously (Gerdil, 1960). The dihedral angle between the benzene ring (C4—C9) and imidazolidine ring (C1—C3/N1/N2) is 6.0 (4) °. In the crystal packing, intermolecular N—H···O hydrogen bonding between centrosymmetrically related molecules lead to loosely associated dimeric aggregates, Table 1. These aggregates are connected into the 3-D crystal structure by C—H···O and π–π interactions, the latter occurring between the imidazolidine and benzene rings, Table 1.

S2. Experimental

Compound (I) (1.13 g, 55% yield) was prepared according to the reported procedure of (Niwata *et al.*, 1997), using 1-(4-methoxyphenyl)urea (0.010 mol; Kurzer *et al.*, 1963), sodium hydride (0.022 mol), *N*,*N*-dimethylformamide (20 ml), and ethyl chloroacetate (0.0120 mol. Colourless single crystals suitable for X-ray diffraction analysis were obtained by recrystallization from a mixture of methanol and water (1:1 V/V).

S3. Refinement

All C-bound H atoms were found on difference maps, but included in the final cycles of refinement using a riding model with C—H = 0.95–0.99 Å, and with U_{iso}(H) = 1.2U_{eq}(C) for aryl- and methylene-H atoms, and 1.5U_{eq}(C) for the methyl H atoms. The N–H1 atom was refined freely.

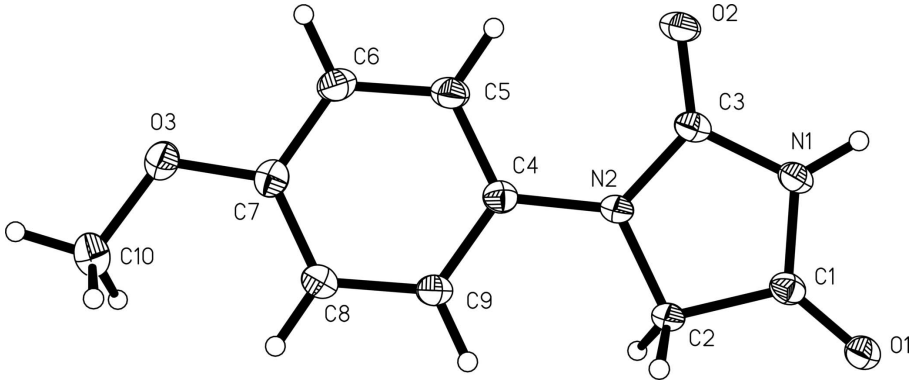

Figure 1

View of the title compound showing atom labelling, with displacement ellipsoids drawn at the 40% probability level.

1-(4-Methoxyphenyl)imidazolidine-2,4-dione

Crystal data

$C_{10}H_{10}N_2O_3$
$M_r = 206.20$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 4.9993$ (10) Å
$b = 6.1566$ (12) Å
$c = 30.052$ (6) Å
$\beta = 93.91$ (3)°
$V = 922.8$ (3) Å^3
$Z = 4$
$F(000) = 432$
$D_x = 1.484$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 196 reflections
$\theta = 2.0$–$27.9°$
$\mu = 0.11$ mm^{-1}
$T = 113$ K
Prism, colourless
0.24 × 0.12 × 0.10 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.974$, $T_{max} = 0.989$
6955 measured reflections
2203 independent reflections
1507 reflections with $I > 2\sigma(I)$
$R_{int} = 0.078$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.7°$
$h = -6\rightarrow4$
$k = -8\rightarrow7$
$l = -34\rightarrow39$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.151$
$S = 1.05$
2203 reflections
142 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
$w = 1/[\sigma^2(F_o^2) + (0.0718P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 1.95 (8)

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. 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.1590 (2)	0.2744 (2)	0.50596 (4)	0.0270 (4)
O2	0.4023 (2)	−0.2177 (2)	0.40235 (4)	0.0286 (4)

O3	1.2460 (3)	0.2947 (2)	0.28363 (4)	0.0303 (4)
N1	0.2393 (3)	−0.0069 (2)	0.45821 (5)	0.0232 (4)
N2	0.5536 (3)	0.1341 (2)	0.41800 (5)	0.0217 (4)
C1	0.2749 (3)	0.1953 (3)	0.47530 (6)	0.0221 (4)
C2	0.4866 (3)	0.3027 (3)	0.44955 (5)	0.0213 (4)
H2A	0.4155	0.4340	0.4338	0.026*
H2B	0.6448	0.3433	0.4694	0.026*
C3	0.4027 (3)	−0.0471 (3)	0.42284 (6)	0.0221 (4)
C4	0.7341 (3)	0.1737 (3)	0.38439 (5)	0.0209 (4)
C5	0.7790 (3)	0.0195 (3)	0.35134 (6)	0.0265 (4)
H5	0.6900	−0.1168	0.3514	0.032*
C6	0.9526 (3)	0.0659 (3)	0.31876 (6)	0.0272 (5)
H6	0.9814	−0.0391	0.2964	0.033*
C7	1.0854 (3)	0.2637 (3)	0.31826 (6)	0.0236 (4)
C8	1.0464 (3)	0.4155 (3)	0.35116 (6)	0.0244 (4)
H8	1.1385	0.5505	0.3513	0.029*
C9	0.8710 (3)	0.3692 (3)	0.38415 (6)	0.0230 (4)
H9	0.8452	0.4735	0.4068	0.028*
C10	1.3963 (4)	0.4914 (3)	0.28380 (7)	0.0339 (5)
H10A	1.2732	0.6153	0.2811	0.051*
H10B	1.5108	0.4915	0.2586	0.051*
H10C	1.5082	0.5027	0.3118	0.051*
H1	0.113 (3)	−0.100 (3)	0.4673 (7)	0.045 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0294 (7)	0.0210 (8)	0.0312 (7)	−0.0022 (5)	0.0070 (5)	−0.0019 (6)
O2	0.0365 (7)	0.0170 (8)	0.0321 (7)	−0.0036 (5)	0.0020 (5)	−0.0035 (5)
O3	0.0331 (7)	0.0295 (9)	0.0295 (7)	−0.0001 (5)	0.0103 (5)	−0.0008 (6)
N1	0.0260 (7)	0.0171 (9)	0.0264 (8)	−0.0035 (5)	0.0012 (6)	0.0003 (6)
N2	0.0269 (8)	0.0151 (8)	0.0232 (8)	−0.0022 (5)	0.0035 (6)	−0.0020 (6)
C1	0.0243 (8)	0.0183 (10)	0.0231 (8)	−0.0002 (6)	−0.0027 (6)	0.0020 (7)
C2	0.0263 (8)	0.0152 (9)	0.0226 (9)	−0.0019 (6)	0.0031 (6)	−0.0019 (7)
C3	0.0253 (8)	0.0171 (10)	0.0235 (9)	−0.0010 (6)	−0.0022 (6)	0.0001 (7)
C4	0.0226 (8)	0.0184 (10)	0.0212 (8)	0.0021 (6)	−0.0006 (6)	0.0015 (7)
C5	0.0320 (9)	0.0181 (10)	0.0295 (10)	−0.0007 (7)	0.0022 (7)	−0.0018 (7)
C6	0.0339 (10)	0.0229 (10)	0.0249 (9)	0.0025 (7)	0.0026 (7)	−0.0038 (8)
C7	0.0219 (9)	0.0259 (11)	0.0229 (9)	0.0041 (6)	0.0011 (6)	0.0022 (7)
C8	0.0256 (9)	0.0216 (10)	0.0259 (9)	−0.0029 (6)	−0.0004 (7)	0.0004 (7)
C9	0.0267 (9)	0.0193 (10)	0.0226 (8)	−0.0008 (6)	−0.0001 (6)	−0.0020 (7)
C10	0.0310 (10)	0.0359 (13)	0.0353 (11)	−0.0048 (8)	0.0067 (8)	0.0036 (9)

Geometric parameters (Å, º)

O1—C1	1.223 (2)	C4—C9	1.385 (2)
O2—C3	1.217 (2)	C4—C5	1.403 (2)
O3—C7	1.370 (2)	C5—C6	1.382 (2)

O3—C10	1.425 (2)	C5—H5	0.9500
N1—C1	1.354 (2)	C6—C7	1.388 (3)
N1—C3	1.406 (2)	C6—H6	0.9500
N1—H1	0.911 (10)	C7—C8	1.384 (2)
N2—C3	1.360 (2)	C8—C9	1.397 (2)
N2—C4	1.420 (2)	C8—H8	0.9500
N2—C2	1.460 (2)	C9—H9	0.9500
C1—C2	1.506 (2)	C10—H10A	0.9800
C2—H2A	0.9900	C10—H10B	0.9800
C2—H2B	0.9900	C10—H10C	0.9800

C7—O3—C10	116.85 (14)	C6—C5—C4	120.02 (17)
C1—N1—C3	112.37 (14)	C6—C5—H5	120.0
C1—N1—H1	122.9 (15)	C4—C5—H5	120.0
C3—N1—H1	124.5 (15)	C5—C6—C7	120.87 (17)
C3—N2—C4	126.92 (15)	C5—C6—H6	119.6
C3—N2—C2	111.09 (14)	C7—C6—H6	119.6
C4—N2—C2	121.66 (14)	O3—C7—C8	124.53 (17)
O1—C1—N1	126.52 (17)	O3—C7—C6	115.84 (16)
O1—C1—C2	126.75 (17)	C8—C7—C6	119.62 (16)
N1—C1—C2	106.72 (15)	C7—C8—C9	119.67 (17)
N2—C2—C1	102.84 (14)	C7—C8—H8	120.2
N2—C2—H2A	111.2	C9—C8—H8	120.2
C1—C2—H2A	111.2	C4—C9—C8	121.02 (16)
N2—C2—H2B	111.2	C4—C9—H9	119.5
C1—C2—H2B	111.2	C8—C9—H9	119.5
H2A—C2—H2B	109.1	O3—C10—H10A	109.5
O2—C3—N2	129.43 (17)	O3—C10—H10B	109.5
O2—C3—N1	123.60 (16)	H10A—C10—H10B	109.5
N2—C3—N1	106.95 (14)	O3—C10—H10C	109.5
C9—C4—C5	118.78 (16)	H10A—C10—H10C	109.5
C9—C4—N2	119.40 (15)	H10B—C10—H10C	109.5
C5—C4—N2	121.82 (16)		

C3—N1—C1—O1	179.61 (16)	C3—N2—C4—C5	−0.8 (3)
C3—N1—C1—C2	−0.94 (18)	C2—N2—C4—C5	−173.66 (15)
C3—N2—C2—C1	1.19 (18)	C9—C4—C5—C6	−1.4 (2)
C4—N2—C2—C1	175.05 (14)	N2—C4—C5—C6	178.85 (15)
O1—C1—C2—N2	179.32 (16)	C4—C5—C6—C7	0.3 (3)
N1—C1—C2—N2	−0.13 (17)	C10—O3—C7—C8	4.6 (2)
C4—N2—C3—O2	6.1 (3)	C10—O3—C7—C6	−176.52 (15)
C2—N2—C3—O2	179.53 (17)	C5—C6—C7—O3	−178.02 (15)
C4—N2—C3—N1	−175.22 (14)	C5—C6—C7—C8	0.9 (3)
C2—N2—C3—N1	−1.77 (19)	O3—C7—C8—C9	177.92 (14)
C1—N1—C3—O2	−179.49 (15)	C6—C7—C8—C9	−0.9 (2)
C1—N1—C3—N2	1.71 (19)	C5—C4—C9—C8	1.4 (3)
C3—N2—C4—C9	179.43 (16)	N2—C4—C9—C8	−178.85 (14)
C2—N2—C4—C9	6.6 (2)	C7—C8—C9—C4	−0.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.91 (1)	1.95 (1)	2.8512 (19)	172 (2)
C2—H2*A*···O2^{ii}	0.99	2.34	3.291 (2)	160
C8—H8···O2^{iii}	0.95	2.42	3.203 (2)	140
*Cg*1···*Cg*1^{iv}			3.705 (3)	
*Cg*1···*Cg*2^{v}			3.622 (3)	

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