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# 1-(4-Methoxyphenyl)pyrrolidine-2,5-dione

**Muhammad Sirajuddin* and Saqib Ali**

Department of Chemistry, Quaid-i-Azam University, Islamabad, Pakistan
Correspondence e-mail: m.siraj09@yahoo.com

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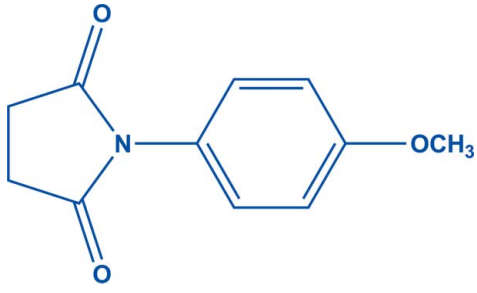
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.034; $wR$ factor = 0.094; data-to-parameter ratio = 14.0.

In the title compound, $C_{11}H_{11}NO_3$, the dihydrofuran-2,5-dione ring has a shallow envelope conformation, with one of the methylene C atoms displaced by 0.216 (1) Å from the other atoms. These near-planar atoms subtend a dihedral angle of 55.88 (8)° with the benzene ring. In the crystal, C—H···O hydrogen bonds link the molecules into [010] chains.

## Related literature

For related structures, see: Sirajuddin *et al.* (2012); Tahir *et al.* (2012).




## Experimental

### Crystal data

$C_{11}H_{11}NO_3$
$M_r$ = 205.21
Monoclinic, $P2_1/n$
$a$ = 9.3684 (7) Å
$b$ = 6.6146 (4) Å
$c$ = 16.0720 (11) Å
$\beta$ = 99.939 (4)°
$V$ = 981.01 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 296 K
0.32 × 0.25 × 0.22 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.968, $T_{max}$ = 0.978
7585 measured reflections
1927 independent reflections
1626 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.094
$S$ = 1.04
1927 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 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···$A$ |
|---|---|---|---|---|
| C2—H2···O3$^{i}$ | 0.93 | 2.50 | 3.1666 (17) | 129 |
| C5—H5···O2$^{ii}$ | 0.93 | 2.47 | 3.3245 (17) | 152 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

The authors acknowledge Quaid-i-Azam University, Islamabad, Pakistan, for providing research facilities, and the University Research Fund (URF) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7117).

## References

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sirajuddin, M., Ali, S. & Tahir, M. N. (2012). *Acta Cryst.* E**68**, o2282.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Tahir, M. N., Sirajuddin, M., Ali, S. & Munawar, K. S. (2012). *Acta Cryst.* E**68**, o2589.

# supporting information

*Acta Cryst.* (2013). E**69**, o1439 [doi:10.1107/S1600536813022460]

## 1-(4-Methoxyphenyl)pyrrolidine-2,5-dione

**Muhammad Sirajuddin and Saqib Ali**

### S1. Experimental

Equimolar quantities of 4-methoxyaniline and dihydrofuran-2,5-dione were stirred and refluxed in acetic acid for 4 h. The solution was kept at room temperature for 24 h which afforded colourless prisms of the title compound.

### S2. Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = xU_{eq}(C)$, where $x$ = 1.5 for methyl and $x$ = 1.2 for other H atoms.

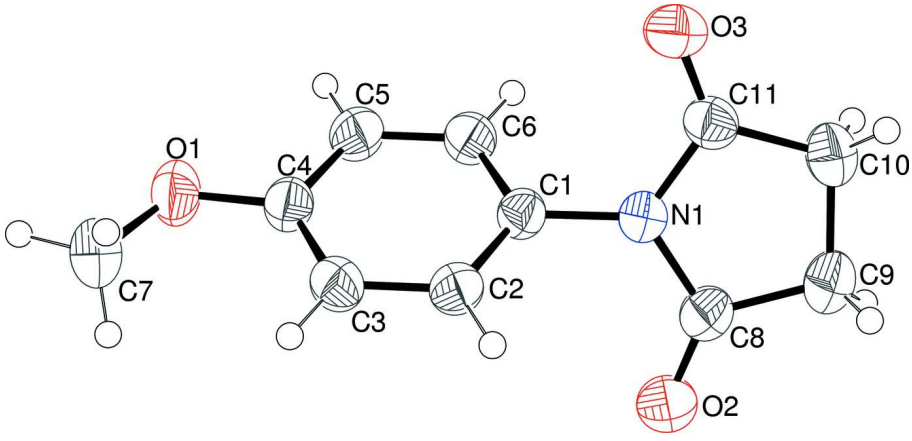



**Figure 1**

View of the title compound with displacement ellipsoids drawn at the 50% probability level.

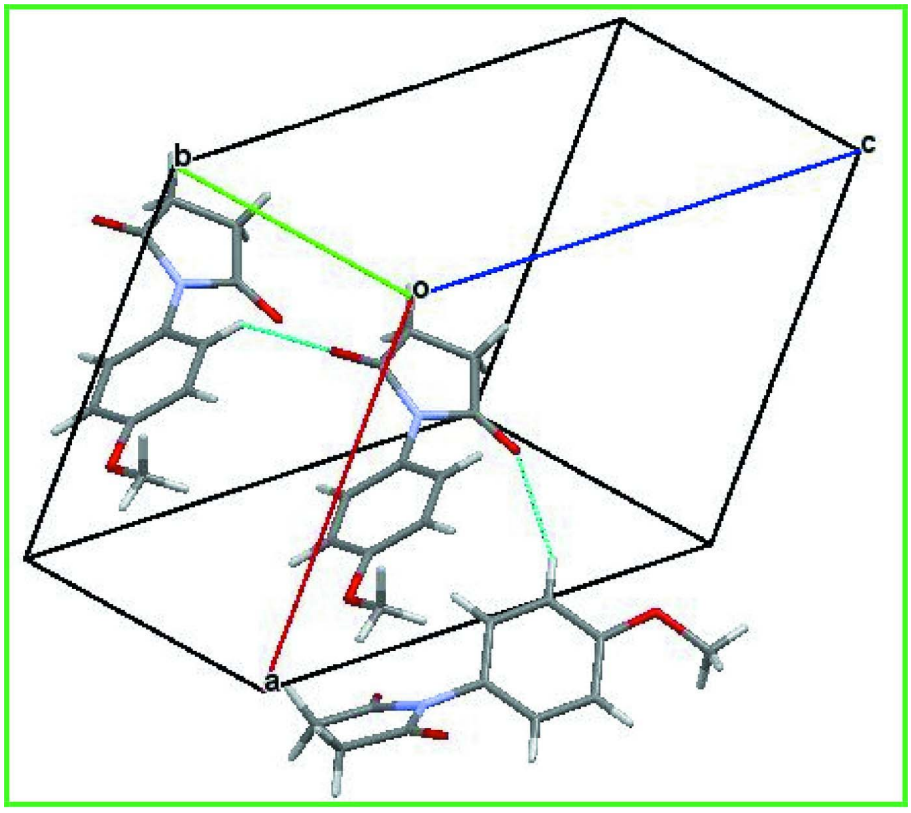



**Figure 2**

The partial packing, which shows that molecules form dimers due to C—H···O bondings.

### 1-(4-Methoxyphenyl)pyrrolidine-2,5-dione

*Crystal data*

$C_{11}H_{11}NO_3$
$M_r = 205.21$
Monoclinic, $P2_1/n$
$a = 9.3684\ (7)$ Å
$b = 6.6146\ (4)$ Å
$c = 16.0720\ (11)$ Å
$\beta = 99.939\ (4)°$
$V = 981.01\ (12)$ Å$^3$
$Z = 4$
$F(000) = 432$
$D_x = 1.389$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\mu = 0.10$ mm$^{-1}$
$T = 296$ K
Prism, colourless
0.32 × 0.25 × 0.22 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 8 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.968$, $T_{max} = 0.978$
7585 measured reflections
1927 independent reflections
1626 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.4°$
$h = -11 \rightarrow 11$
$k = -8 \rightarrow 7$
$l = -19 \rightarrow 19$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.094$
$S = 1.04$
1927 reflections
138 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.2498P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å$^{-3}$
$\Delta\rho_{min} = -0.14$ e Å$^{-3}$
Extinction correction: *SHELXL2012* (Sheldrick, 2012), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.047 (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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.73798 (12) | −0.12759 (16) | 0.03467 (7) | 0.0594 (3) |
| O2 | 0.52321 (14) | −0.03671 (17) | 0.38782 (7) | 0.0685 (4) |
| O3 | 0.38050 (12) | 0.48906 (15) | 0.21179 (6) | 0.0588 (3) |
| N1 | 0.48031 (11) | 0.21443 (15) | 0.28804 (6) | 0.0397 (3) |
| C1 | 0.54572 (13) | 0.12100 (19) | 0.22333 (7) | 0.0378 (3) |
| C2 | 0.50543 (14) | −0.0707 (2) | 0.19526 (8) | 0.0418 (3) |
| H2 | 0.4367 | −0.1412 | 0.2192 | 0.050* |
| C3 | 0.56658 (14) | −0.1592 (2) | 0.13165 (8) | 0.0441 (3) |
| H3 | 0.5385 | −0.2882 | 0.1125 | 0.053* |
| C4 | 0.66963 (14) | −0.0546 (2) | 0.09689 (8) | 0.0427 (3) |
| C5 | 0.71239 (14) | 0.1368 (2) | 0.12663 (9) | 0.0461 (3) |
| H5 | 0.7830 | 0.2061 | 0.1039 | 0.055* |
| C6 | 0.65080 (14) | 0.2246 (2) | 0.18962 (8) | 0.0427 (3) |
| H6 | 0.6797 | 0.3529 | 0.2094 | 0.051* |
| C7 | 0.6833 (2) | −0.3084 (2) | −0.00666 (10) | 0.0639 (4) |
| H7A | 0.6941 | −0.4177 | 0.0333 | 0.096* |
| H7B | 0.7362 | −0.3386 | −0.0512 | 0.096* |
| H7C | 0.5825 | −0.2911 | −0.0299 | 0.096* |
| C8 | 0.47536 (15) | 0.1275 (2) | 0.36638 (8) | 0.0471 (3) |
| C9 | 0.39873 (18) | 0.2721 (2) | 0.41557 (9) | 0.0556 (4) |
| H9A | 0.4574 | 0.3009 | 0.4701 | 0.067* |
| H9B | 0.3067 | 0.2164 | 0.4244 | 0.067* |
| C10 | 0.37563 (16) | 0.4609 (2) | 0.36233 (9) | 0.0494 (4) |
| H10A | 0.2764 | 0.5078 | 0.3572 | 0.059* |
| H10B | 0.4402 | 0.5679 | 0.3869 | 0.059* |
| C11 | 0.40880 (14) | 0.39934 (19) | 0.27787 (8) | 0.0418 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0720 (7) | 0.0563 (6) | 0.0574 (6) | −0.0022 (5) | 0.0327 (5) | −0.0108 (5) |
| O2 | 0.0974 (9) | 0.0604 (7) | 0.0501 (6) | 0.0251 (6) | 0.0192 (6) | 0.0146 (5) |
| O3 | 0.0802 (7) | 0.0454 (6) | 0.0510 (6) | 0.0083 (5) | 0.0116 (5) | 0.0074 (5) |
| N1 | 0.0446 (6) | 0.0388 (6) | 0.0366 (6) | 0.0017 (4) | 0.0099 (4) | −0.0006 (4) |
| C1 | 0.0399 (6) | 0.0397 (6) | 0.0337 (6) | 0.0018 (5) | 0.0065 (5) | −0.0006 (5) |
| C2 | 0.0427 (7) | 0.0406 (7) | 0.0440 (7) | −0.0038 (5) | 0.0125 (5) | 0.0014 (5) |
| C3 | 0.0488 (7) | 0.0380 (7) | 0.0458 (7) | −0.0034 (6) | 0.0090 (6) | −0.0048 (6) |
| C4 | 0.0447 (7) | 0.0458 (7) | 0.0388 (7) | 0.0036 (6) | 0.0110 (5) | −0.0010 (6) |
| C5 | 0.0450 (7) | 0.0468 (8) | 0.0494 (8) | −0.0058 (6) | 0.0163 (6) | 0.0017 (6) |
| C6 | 0.0453 (7) | 0.0392 (7) | 0.0436 (7) | −0.0054 (5) | 0.0079 (5) | −0.0033 (5) |
| C7 | 0.0837 (11) | 0.0598 (10) | 0.0514 (9) | 0.0052 (8) | 0.0207 (8) | −0.0129 (7) |
| C8 | 0.0540 (8) | 0.0498 (8) | 0.0377 (7) | 0.0036 (6) | 0.0088 (6) | 0.0021 (6) |
| C9 | 0.0657 (9) | 0.0614 (9) | 0.0430 (8) | 0.0048 (7) | 0.0183 (7) | −0.0035 (7) |
| C10 | 0.0496 (8) | 0.0492 (8) | 0.0502 (8) | 0.0003 (6) | 0.0110 (6) | −0.0116 (6) |
| C11 | 0.0440 (7) | 0.0363 (6) | 0.0447 (7) | −0.0034 (5) | 0.0066 (5) | −0.0023 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C4 | 1.3654 (16) | C5—C6 | 1.3773 (18) |
| O1—C7 | 1.4203 (18) | C5—H5 | 0.9300 |
| O2—C8 | 1.2028 (17) | C6—H6 | 0.9300 |
| O3—C11 | 1.2055 (16) | C7—H7A | 0.9600 |
| N1—C11 | 1.3905 (16) | C7—H7B | 0.9600 |
| N1—C8 | 1.3920 (17) | C7—H7C | 0.9600 |
| N1—C1 | 1.4350 (15) | C8—C9 | 1.5002 (19) |
| C1—C2 | 1.3766 (18) | C9—C10 | 1.508 (2) |
| C1—C6 | 1.3844 (18) | C9—H9A | 0.9700 |
| C2—C3 | 1.3850 (18) | C9—H9B | 0.9700 |
| C2—H2 | 0.9300 | C10—C11 | 1.5003 (18) |
| C3—C4 | 1.3819 (18) | C10—H10A | 0.9700 |
| C3—H3 | 0.9300 | C10—H10B | 0.9700 |
| C4—C5 | 1.3873 (19) | | |
| | | | |
| C4—O1—C7 | 117.61 (11) | O1—C7—H7B | 109.5 |
| C11—N1—C8 | 112.27 (11) | H7A—C7—H7B | 109.5 |
| C11—N1—C1 | 123.43 (10) | O1—C7—H7C | 109.5 |
| C8—N1—C1 | 124.25 (11) | H7A—C7—H7C | 109.5 |
| C2—C1—C6 | 120.06 (11) | H7B—C7—H7C | 109.5 |
| C2—C1—N1 | 120.46 (11) | O2—C8—N1 | 124.27 (13) |
| C6—C1—N1 | 119.47 (11) | O2—C8—C9 | 127.83 (13) |
| C1—C2—C3 | 120.42 (12) | N1—C8—C9 | 107.89 (12) |
| C1—C2—H2 | 119.8 | C8—C9—C10 | 105.29 (11) |
| C3—C2—H2 | 119.8 | C8—C9—H9A | 110.7 |
| C4—C3—C2 | 119.58 (12) | C10—C9—H9A | 110.7 |
| C4—C3—H3 | 120.2 | C8—C9—H9B | 110.7 |

| | | | |
|---|---|---|---|
| C2—C3—H3 | 120.2 | C10—C9—H9B | 110.7 |
| O1—C4—C3 | 124.58 (12) | H9A—C9—H9B | 108.8 |
| O1—C4—C5 | 115.53 (12) | C11—C10—C9 | 104.87 (11) |
| C3—C4—C5 | 119.87 (12) | C11—C10—H10A | 110.8 |
| C6—C5—C4 | 120.36 (12) | C9—C10—H10A | 110.8 |
| C6—C5—H5 | 119.8 | C11—C10—H10B | 110.8 |
| C4—C5—H5 | 119.8 | C9—C10—H10B | 110.8 |
| C5—C6—C1 | 119.69 (12) | H10A—C10—H10B | 108.8 |
| C5—C6—H6 | 120.2 | O3—C11—N1 | 124.39 (12) |
| C1—C6—H6 | 120.2 | O3—C11—C10 | 127.96 (13) |
| O1—C7—H7A | 109.5 | N1—C11—C10 | 107.65 (11) |
| | | | |
| C11—N1—C1—C2 | −123.12 (13) | N1—C1—C6—C5 | −179.05 (11) |
| C8—N1—C1—C2 | 53.95 (17) | C11—N1—C8—O2 | 176.06 (14) |
| C11—N1—C1—C6 | 57.37 (16) | C1—N1—C8—O2 | −1.3 (2) |
| C8—N1—C1—C6 | −125.55 (14) | C11—N1—C8—C9 | −2.76 (16) |
| C6—C1—C2—C3 | −1.76 (19) | C1—N1—C8—C9 | 179.88 (12) |
| N1—C1—C2—C3 | 178.74 (11) | O2—C8—C9—C10 | 174.72 (15) |
| C1—C2—C3—C4 | 0.6 (2) | N1—C8—C9—C10 | −6.52 (16) |
| C7—O1—C4—C3 | 10.8 (2) | C8—C9—C10—C11 | 12.49 (15) |
| C7—O1—C4—C5 | −170.72 (13) | C8—N1—C11—O3 | −168.93 (13) |
| C2—C3—C4—O1 | 179.31 (12) | C1—N1—C11—O3 | 8.5 (2) |
| C2—C3—C4—C5 | 0.8 (2) | C8—N1—C11—C10 | 11.02 (15) |
| O1—C4—C5—C6 | −179.76 (12) | C1—N1—C11—C10 | −171.59 (11) |
| C3—C4—C5—C6 | −1.2 (2) | C9—C10—C11—O3 | 165.50 (14) |
| C4—C5—C6—C1 | 0.0 (2) | C9—C10—C11—N1 | −14.44 (14) |
| C2—C1—C6—C5 | 1.44 (19) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···O3$^{i}$ | 0.93 | 2.50 | 3.1666 (17) | 129 |
| C5—H5···O2$^{ii}$ | 0.93 | 2.47 | 3.3245 (17) | 152 |

Symmetry codes: (i) $x$, $y-1$, $z$; (ii) $-x+3/2$, $y+1/2$, $-z+1/2$.