Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(Morpholin-4-ylmethyl)pyrrolidine-2,5-dione

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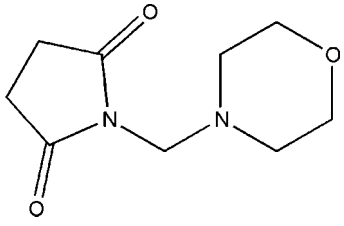
Received 15 September 2007; accepted 19 September 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.089; data-to-parameter ratio = 13.6.

In the title compound, $C_9H_{14}N_2O_3$, the morpholine ring adopts the usual chair conformation. The pyrrolidine-2,5-dione ring adopts an extremely flattened envelope conformation. The crystal structure is stabilized by weak C—H···O interactions.

Related literature

For related literature, see: Allen (2002); Allen *et al.* (1987); Fisher & Wyvratt (1990); Li *et al.* (1998); Lucka-Sobstel *et al.* (1977); Ramnathan *et al.* (1996); Yoshioka (1995); Zejc & Obniska (1984).



Experimental

Crystal data

$C_9H_{14}N_2O_3$
M_r = 198.22
Monoclinic, $P2_1/n$
a = 6.1368 (2) Å
b = 7.8038 (3) Å
c = 20.9032 (8) Å
β = 98.202 (2)°
V = 990.82 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.26 × 0.18 × 0.18 mm

Data collection

Bruker Kappa-APEX2 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.974, T_{max} = 0.982
8190 measured reflections
1726 independent reflections
1184 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.089
S = 1.01
1726 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2B···O2^{i}	0.97	2.33	3.265 (2)	162
C5—H5B···O1	0.97	2.56	2.886 (2)	100

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-NT* (Bruker, 2004); data reduction: *SAINT-NT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *PLATON* (Spek, 2003).

The authours thank Professor A. Sebastiyan for providing the sample to carry out X-ray studies.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2514).

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supplementary materials

Acta Cryst. (2007). E**63**, o4143 [**doi:10.1107/S1600536807046053**]

1-(Morpholin-4-ylmethyl)pyrrolidine-2,5-dione

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Comment

Morpholine is a multipurpose chemical which is used as a solvent for resins, dyes and waxes. One of its most important uses is as a chemical intermediate in the preparation of pesticides (Li *et al.*, 1998). Drugs containing a morpholine ring have established activities that include the reduction of blood sugar and lipid levels (Yoshioka, 1995), and amelioration of obesity and insulin resistance (Fisher & Wyvratt, 1990). Owing to their pharmcological activities these compounds have received a great deal of attention in respect of their synthesis and conformation. A group of phenylsuccinimides (Lucka-Sobstel Zejc & Obniska 1977; Zejc & Obniska, 1984) proved to have strong anticonvulsive activity.

A perspective view of the title compound is shown in Fig. 1. In the morpholine ring, the average C—N, C—C and C—O bond distances [1.453 (2), 1.497 (2) and 1.417 (2) A°, respectively] are in good agreement with earlier reports (Ramnathan *et al.*, 1996). The morpholine ring adopts the usual chair conformation. This is in agreement with the structural data available from Version 5.14 of the Cambridge Structural Database (Allen, 2002). The pyrrolidine-2,5-dione or succinimide ring adopts an extremely flattened envelope conformation with atom C1 deviating by 0.025 A° from the mean plane through the remaining atoms in the ring. The sum of the angles around N1 is 358.70 (13)° indicating sp^2 hybridization. However the N1—C1 [1.3870 (2)Å and N1—C4 [1.375 (19) Å] distances are intermediate between the average C_{ar} –Nsp^3(pyramidal) [1.419 (17) Å] and C_{ar}—Nsp^2(planar) [1.353 (7) Å] distances reported by Allen *et al.* (1987). The dihedral angle between the planes of the morpholine and pyrrolidine-2,5-dione ring is 63.26 (7)°. Weak intermolecular C—H···O (Fig 2) interactions stabilize the crystal packing.

Experimental

The title compound was synthesized by condensing morpholine, formaldehyde and succinimide. Then, 9.9 g (0.1*M*) of succinimide was stirred with 8.1 g of 37% acqueous formaldehyde until the solid succinimide had dissolved. Morpholine (8.0 ml, 0.1*M*) was added in small quantities and stirred well. The mixture turned oily and was allowed to stand at room temperature for about 12 h. The colorless crystalline product was sepearated by filtration. The crude product was recrystallized from a mixture of ethanol and acetone. Melting point 98°C.

Figures

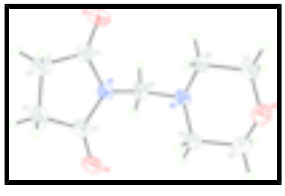

Fig. 1. The structure of the title compound, showing the atom numbering scheme with 50% probability displacement ellipsoids.

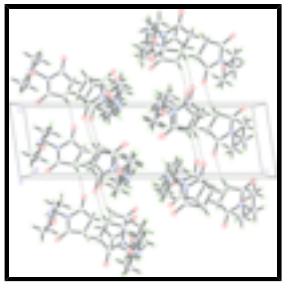

Fig. 2. Packing diagram of the title compound. C—H···O interactions are drawn as dashed lines.

1-(Morpholin-4-ylmethyl)pyrrolidine-2,5-dione

Crystal data

$C_9H_{14}N_2O_3$	F_{000} = 424
M_r = 198.22	D_x = 1.329 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2548 reflections
a = 6.1368 (2) Å	θ = 2.0–23.7º
b = 7.8038 (3) Å	μ = 0.10 mm^{-1}
c = 20.9032 (8) Å	T = 293 (2) K
β = 98.202 (2)º	Prism, colourless
V = 990.82 (6) Å^3	0.26 × 0.18 × 0.18 mm
Z = 4	

Data collection

Bruker Kappa-APEX2 diffractometer	1726 independent reflections
Radiation source: fine focus sealed tube	1184 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 293(2) K	θ_{max} = 25º
ω and φ scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Bruker, 2004)	h = −6→6
T_{min} = 0.974, T_{max} = 0.982	k = −6→8
8190 measured reflections	l = −23→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.033	H-atom parameters constrained
$wR(F^2)$ = 0.089	$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.1664P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$

1726 reflections	$\Delta\rho_{max} = 0.12$ e Å^{-3}
127 parameters	$\Delta\rho_{min} = -0.13$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.0573 (2)	0.26782 (18)	0.07851 (6)	0.0734 (5)
O2	0.6854 (2)	0.35020 (16)	0.21769 (5)	0.0655 (5)
O3	0.4045 (2)	0.94347 (16)	0.10318 (6)	0.0763 (5)
N1	0.3883 (2)	0.33660 (15)	0.13812 (5)	0.0409 (4)
N2	0.4843 (2)	0.59584 (16)	0.07942 (5)	0.0417 (4)
C1	0.1818 (3)	0.2607 (2)	0.12828 (8)	0.0517 (6)
C2	0.1444 (3)	0.1732 (3)	0.18956 (9)	0.0658 (7)
C3	0.3581 (3)	0.1936 (2)	0.23465 (8)	0.0621 (7)
C4	0.5006 (3)	0.3011 (2)	0.19838 (7)	0.0467 (6)
C5	0.4923 (3)	0.4132 (2)	0.08505 (7)	0.0465 (6)
C6	0.2643 (3)	0.6669 (2)	0.06615 (7)	0.0487 (6)
C7	0.2771 (3)	0.8541 (2)	0.05144 (9)	0.0636 (7)
C8	0.6188 (3)	0.8747 (3)	0.11511 (10)	0.0714 (8)
C9	0.6152 (3)	0.6885 (2)	0.13172 (7)	0.0514 (6)
H2A	0.11023	0.05294	0.18181	0.0790*
H2B	0.02398	0.22664	0.20757	0.0790*
H3A	0.33333	0.25000	0.27434	0.0746*
H3B	0.42567	0.08294	0.24526	0.0746*
H5A	0.64555	0.37833	0.09061	0.0558*
H5B	0.42212	0.36475	0.04455	0.0558*
H6A	0.18837	0.65066	0.10335	0.0585*
H6B	0.18165	0.60800	0.02962	0.0585*
H7A	0.34281	0.86915	0.01228	0.0762*
H7B	0.12965	0.90176	0.04402	0.0762*
H8A	0.70361	0.93659	0.15048	0.0857*
H8B	0.69063	0.88966	0.07704	0.0857*
H9A	0.76414	0.64376	0.13844	0.0616*
H9B	0.55246	0.67330	0.17139	0.0616*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0646 (9)	0.0780 (10)	0.0687 (8)	−0.0037 (7)	−0.0209 (7)	0.0066 (7)
O2	0.0579 (9)	0.0811 (10)	0.0524 (7)	0.0013 (7)	−0.0095 (6)	0.0102 (6)
O3	0.0862 (10)	0.0493 (8)	0.0854 (9)	0.0096 (7)	−0.0156 (7)	−0.0157 (6)
N1	0.0463 (8)	0.0413 (8)	0.0339 (6)	0.0048 (6)	0.0012 (5)	0.0019 (5)
N2	0.0479 (8)	0.0437 (8)	0.0327 (6)	0.0038 (6)	0.0032 (5)	0.0010 (5)
C1	0.0504 (10)	0.0460 (11)	0.0562 (10)	0.0050 (8)	−0.0013 (8)	−0.0005 (8)
C2	0.0614 (12)	0.0686 (13)	0.0694 (11)	−0.0025 (9)	0.0158 (9)	0.0113 (9)
C3	0.0763 (13)	0.0628 (12)	0.0479 (10)	0.0004 (9)	0.0110 (9)	0.0119 (8)
C4	0.0515 (11)	0.0473 (10)	0.0395 (8)	0.0094 (8)	0.0000 (7)	0.0010 (7)
C5	0.0575 (10)	0.0492 (11)	0.0335 (8)	0.0083 (8)	0.0089 (7)	−0.0018 (7)
C6	0.0508 (10)	0.0512 (11)	0.0407 (8)	0.0037 (8)	−0.0053 (7)	0.0007 (7)
C7	0.0703 (13)	0.0510 (12)	0.0633 (11)	0.0097 (9)	−0.0113 (9)	−0.0007 (8)
C8	0.0716 (14)	0.0591 (13)	0.0773 (13)	−0.0117 (10)	−0.0110 (10)	0.0001 (10)
C9	0.0464 (10)	0.0577 (11)	0.0474 (9)	−0.0021 (8)	−0.0022 (7)	0.0008 (8)

Geometric parameters (Å, °)

O1—C1	1.201 (2)	C2—H2A	0.9700
O2—C4	1.211 (2)	C2—H2B	0.9700
O3—C7	1.423 (2)	C3—H3A	0.9700
O3—C8	1.409 (2)	C3—H3B	0.9700
N1—C1	1.387 (2)	C5—H5A	0.9700
N1—C4	1.3750 (19)	C5—H5B	0.9700
N1—C5	1.4823 (19)	C6—H6A	0.9700
N2—C5	1.430 (2)	C6—H6B	0.9700
N2—C6	1.449 (2)	C7—H7A	0.9700
N2—C9	1.4535 (19)	C7—H7B	0.9700
C1—C2	1.498 (3)	C8—H8A	0.9700
C2—C3	1.510 (3)	C8—H8B	0.9700
C3—C4	1.494 (2)	C9—H9A	0.9700
C6—C7	1.497 (2)	C9—H9B	0.9700
C8—C9	1.495 (3)		
O1···C6	3.387 (2)	C6···O1^{i}	3.405 (2)
O1···C7^{i}	3.302 (2)	C6···O1	3.387 (2)
O1···C6^{i}	3.405 (2)	C7···O1^{i}	3.302 (2)
O2···C9	3.1881 (19)	C9···O2	3.1881 (19)
O2···C2^{ii}	3.265 (2)	C9···C4	3.443 (2)
O3···C3^{iii}	3.416 (2)	C1···H6A	3.0900
O3···C1^{iii}	2.911 (2)	C4···H9B	2.9800
O3···C2^{iii}	3.138 (2)	H2A···O3^{vi}	2.7500
O3···N2	2.8134 (18)	H2A···H3A^{viii}	2.5400
O3···N1^{iii}	3.1585 (17)	H2B···O2^{iv}	2.3300
O1···H5A^{iv}	2.7200	H3A···H2A^{ix}	2.5400

O1···H6B^{i}	2.6900	H5A···O1^{ii}	2.7200
O1···H5B	2.5600	H5A···O2	2.6400
O2···H8A^{v}	2.8200	H5A···H9A	2.3700
O2···H9B	2.7800	H5B···O1	2.5600
O2···H2B^{ii}	2.3300	H5B···H6B	2.4000
O2···H5A	2.6400	H5B···N2^{vii}	2.7500
O2···H9A	2.9100	H6A···N1	2.7900
O3···H2A^{iii}	2.7500	H6A···C1	3.0900
N1···O3^{vi}	3.1585 (17)	H6A···H9B	2.4800
N2···O3	2.8134 (18)	H6B···H5B	2.4000
N1···H6A	2.7900	H6B···O1^{i}	2.6900
N1···H9B	2.8600	H7A···H8B	2.3600
N2···H5B^{vii}	2.7500	H8A···O2^{x}	2.8200
C1···O3^{vi}	2.911 (2)	H8B···H7A	2.3600
C1···C6	3.490 (2)	H9A···O2	2.9100
C2···O2^{iv}	3.265 (2)	H9A···H5A	2.3700
C2···O3^{vi}	3.138 (2)	H9B···O2	2.7800
C3···O3^{vi}	3.416 (2)	H9B···N1	2.8600
C4···C9	3.443 (2)	H9B···C4	2.9800
C6···C1	3.490 (2)	H9B···H6A	2.4800
C7—O3—C8	110.21 (14)	C4—C3—H3B	111.00
C1—N1—C4	112.19 (13)	H3A—C3—H3B	109.00
C1—N1—C5	122.88 (12)	N1—C5—H5A	108.00
C4—N1—C5	123.63 (13)	N1—C5—H5B	108.00
C5—N2—C6	114.65 (13)	N2—C5—H5A	108.00
C5—N2—C9	115.15 (12)	N2—C5—H5B	108.00
C6—N2—C9	110.70 (12)	H5A—C5—H5B	107.00
O1—C1—N1	124.29 (15)	N2—C6—H6A	110.00
O1—C1—C2	127.28 (17)	N2—C6—H6B	110.00
N1—C1—C2	108.42 (14)	C7—C6—H6A	110.00
C1—C2—C3	105.09 (15)	C7—C6—H6B	110.00
C2—C3—C4	105.16 (14)	H6A—C6—H6B	108.00
O2—C4—N1	124.40 (15)	O3—C7—H7A	109.00
O2—C4—C3	126.64 (14)	O3—C7—H7B	109.00
N1—C4—C3	108.96 (14)	C6—C7—H7A	109.00
N1—C5—N2	116.74 (13)	C6—C7—H7B	109.00
N2—C6—C7	109.75 (14)	H7A—C7—H7B	108.00
O3—C7—C6	111.18 (14)	O3—C8—H8A	109.00
O3—C8—C9	111.53 (16)	O3—C8—H8B	109.00
N2—C9—C8	109.50 (13)	C9—C8—H8A	109.00
C1—C2—H2A	111.00	C9—C8—H8B	109.00
C1—C2—H2B	111.00	H8A—C8—H8B	108.00
C3—C2—H2A	111.00	N2—C9—H9A	110.00
C3—C2—H2B	111.00	N2—C9—H9B	110.00
H2A—C2—H2B	109.00	C8—C9—H9A	110.00
C2—C3—H3A	111.00	C8—C9—H9B	110.00

C2—C3—H3B	111.00	H9A—C9—H9B	108.00
C4—C3—H3A	111.00		
C7—O3—C8—C9	−58.88 (19)	C9—N2—C6—C7	56.19 (16)
C8—O3—C7—C6	58.47 (19)	C5—N2—C6—C7	−171.49 (12)
C5—N1—C1—O1	−9.5 (2)	C6—N2—C5—N1	−62.17 (16)
C4—N1—C1—O1	−176.91 (16)	C9—N2—C5—N1	68.00 (18)
C1—N1—C4—C3	−1.31 (18)	C6—N2—C9—C8	−56.24 (17)
C4—N1—C1—C2	3.70 (19)	N1—C1—C2—C3	−4.46 (19)
C5—N1—C1—C2	171.08 (14)	O1—C1—C2—C3	176.17 (17)
C4—N1—C5—N2	−92.60 (18)	C1—C2—C3—C4	3.57 (19)
C1—N1—C4—O2	178.49 (15)	C2—C3—C4—N1	−1.57 (18)
C5—N1—C4—O2	11.2 (2)	C2—C3—C4—O2	178.63 (17)
C5—N1—C4—C3	−168.58 (13)	N2—C6—C7—O3	−57.18 (17)
C1—N1—C5—N2	101.46 (17)	O3—C8—C9—N2	57.76 (19)
C5—N2—C9—C8	171.70 (14)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2B···O2^{iv}	0.97	2.33	3.265 (2)	162
C5—H5B···O1	0.97	2.56	2.886 (2)	100

Symmetry codes: (iv) *x*−1, *y*, *z*.

Fig. 1

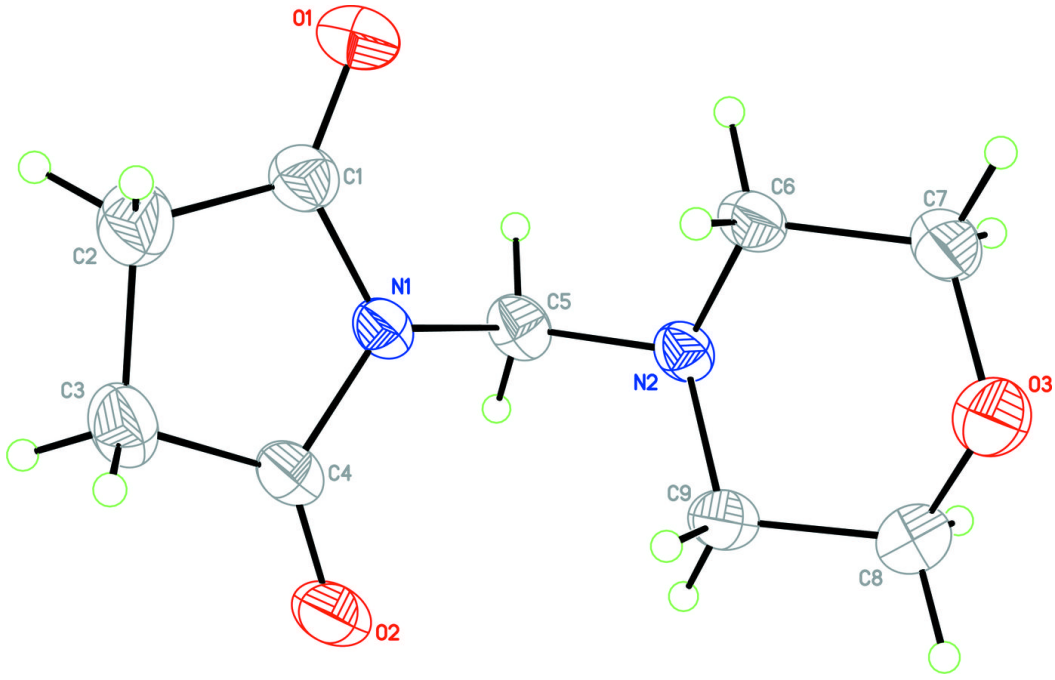

Fig. 2