

## (8a*S*)-8,8a-Dihydrofuro[3,2-*f*]indolizine-6,9(4*H*,7*H*)-dione

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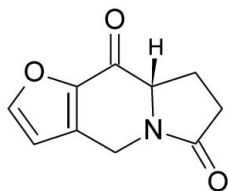
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.120; data-to-parameter ratio = 11.0.

In the title compound,  $\text{C}_{10}\text{H}_9\text{NO}_3$ , the central six-membered ring has an envelope conformation, with the greatest deviation from the mean plane of the ring being 0.452 (2) Å for the bridgehead N atom. The conformation of the fused oxopyrrolidine ring is close to that of a flat envelope, with the greatest deviation being 0.263 (3) Å from the mean plane (for the C atom attached to the non-nitrogen bridgehead in the pyrrolidine ring) defined by other four atoms of the ring. The furan ring attached to the indolizine ring system is nearly coplanar [mean deviation is 0.006 (2) Å]. The crystal structure is stabilized by weak  $\text{C}-\text{H}\cdots\text{O}$  interactions; they seem to be effective in the stabilization of the structure.

### Related literature

For related literature, see: Brandi *et al.* (1995); Brown & Corbridge (1954); Camus *et al.* (2000); Gubin *et al.* (1992); Gundersen *et al.* (2003); Hema *et al.* (2003); Hempel *et al.* (1993); Marchalín *et al.* (1998); Nardelli (1983); Okada *et al.* (1993); Pedersen (1967); Poty *et al.* (1994); Rosseels *et al.* (1982); Vrábek *et al.* (2004).



### Experimental

#### Crystal data

$\text{C}_{10}\text{H}_9\text{NO}_3$	$V = 880.17$ (2) Å <sup>3</sup>
$M_r = 191.18$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 6.8771$ (1) Å	$\mu = 0.11$ mm <sup>-1</sup>
$b = 7.2198$ (1) Å	$T = 298$ (2) K
$c = 17.7271$ (2) Å	$0.51 \times 0.25 \times 0.07$ mm

#### Data collection

Oxford Diffraction Gemini R CCD diffractometer	35953 measured reflections
Absorption correction: analytical (Clark & Reid, 1995)	1409 independent reflections
$T_{\min} = 0.943$ , $T_{\max} = 0.993$	1110 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.027$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	128 parameters
$wR(F^2) = 0.120$	H-atom parameters constrained
$S = 1.03$	$\Delta\rho_{\max} = 0.14$ e Å <sup>-3</sup>
1409 reflections	$\Delta\rho_{\min} = -0.15$ e Å <sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C3}-\text{H3}\cdots\text{O3}^{\text{i}}$	0.93	2.44	3.278 (3)	150
$\text{C2}-\text{H2}\cdots\text{O2}^{\text{ii}}$	0.93	2.64	3.374 (3)	136
$\text{C12}-\text{H12}\cdots\text{O2}^{\text{iii}}$	0.98	2.64	3.344 (3)	129
$\text{C8}-\text{H8B}\cdots\text{O1}^{\text{iv}}$	0.97	2.63	3.547 (3)	157
$\text{C8}-\text{H8A}\cdots\text{O3}^{\text{v}}$	0.97	2.72	3.417 (4)	130

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2027).

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**supplementary materials**

*Acta Cryst.* (2007). E63, o3180–o3181 [ doi:10.1107/S1600536807028176 ]

## (8a*S*)-8,8a-Dihydrofuro[3,2-*f*]indolizine-6,9(4*H*,7*H*)-dione

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### Comment

Indolizine derivatives are an important class of heterocyclic bioactive compounds which have a wide range of applications, such as pharmaceutical drugs, potential central nervous system depressants, calcium entry blockers, cardiovascular agents, spectral sensitizers and novel dyes (Gubin *et al.*, 1992; Poty *et al.*, 1994; Hema *et al.*, 2003). Several polyhydroxylated indolizines are interesting as inhibitors of glycosides (Hempel *et al.*, 1993; Brandi *et al.*, 1995). Indolizines have also been tested as antimycobacterial agents against mycobacterial tuberculosis (Gundersen *et al.*, 2003), for the treatment of angina pectoris (Rosseels *et al.*, 1982) and as testosterone 5 $\alpha$ -reductase inhibitors (Okada *et al.*, 1993). Due to the diverse properties of indolizine derivatives, the structure of the title compound, (I), has been determined as part of our study of the conformational changes caused by different substituents at various positions on the indolizine ring system. The absolute configuration is known from the synthesis and is depicted in the scheme and figure. The bond lengths and bond angles in the molecule are comparable with those in related structures (Camus *et al.*, 2000; Vrábek *et al.*, 2004). The central N-heterocyclic ring is not planar and adopts a chair conformation (Nardelli, 1983). A calculation of least-squares planes shows that this ring is puckered in such a manner that the five atoms C4, C10, C11, C9 and C12 are coplanar to within 0.020 (2) Å, while atom N5 is displaced from this plane with out-of-plane displacement of 0.452 (2) Å. The oxopyrrolidine ring is distorted towards a flat-envelope conformation, with atom C8 on the flap. The deviation of atom C8 from the mean plane of the remaining four atoms is 0.263 (3) Å. The fused furan ring is planar (mean deviation 0.006 (2) Å). The N5—C4 and N5—C12 bonds are approximately equivalent and both are much longer than the N5—C6 bond. Moreover, the N5 atom is *sp*<sup>2</sup> hybridized, as evidenced by the sum of the valence angles around it [360.0 (1)°]. These data are consistent with conjugation of the lone-pair electrons on N5 with the adjacent carbonyl and agree with literature values for simple amides (Brown & Corbridge, 1954; Pedersen, 1967). The bond lengths of the carbonyl groups C9=O2 and C6=O3 are 1.216 (3) and 1.221 (3) Å, respectively, are somewhat longer than typical carbonyl bonds. This may be due to the fact that atoms O2 and O3 participate in intermolecular van der Waals forces.

### Experimental

(*S*)-Glutamic acid was condensed with 3-furaldehyde to give a Schiff base, which upon treatment with sodium borohydride gave the crude (*S*)-*N*-(furylmethyl)-glutamic acid (Marchalín *et al.*, 1998). Cyclization of acid into oxoproline was performed in refluxing ethanol in good yield (75%). This amino acid was conveniently converted to acid chloride by the action of thionyl chloride in dichloromethane. The resulting acid chloride under Friedel-Crafts cyclization conditions using aluminium trichloride of high quality as a catalyst gave the expected ketone in moderate yield (72%); mp 433–435 K.

### Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93 – 0.98 Å and  $U_{\text{iso}}$  set at  $1.2U_{\text{eq}}$  of the parent atom. The absolute configuration could not be

# supplementary materials

reliably determined for this compound using Mo radiation, and has been assigned according to the synthesis; Friedel pairs have been merged.

## Figures

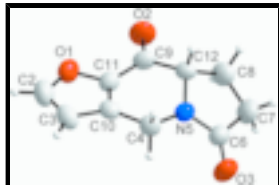


Fig. 1. Molecular structure of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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### Crystal data

$C_{10}H_9NO_3$	$F_{000} = 400$
$M_r = 191.18$	$D_x = 1.443 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
Hall symbol: P 2ac 2ab	$\lambda = 0.71073 \text{ \AA}$
$a = 6.87710 (10) \text{ \AA}$	Cell parameters from 16436 reflections
$b = 7.21980 (10) \text{ \AA}$	$\theta = 3.0\text{--}29.5^\circ$
$c = 17.7271 (2) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$V = 880.17 (2) \text{ \AA}^3$	$T = 298 (2) \text{ K}$
$Z = 4$	Block, yellow
	$0.51 \times 0.25 \times 0.07 \text{ mm}$

### Data collection

Oxford Diffraction Gemini R CCD diffractometer	1409 independent reflections
Radiation source: fine-focus sealed tube	1110 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.027$
Detector resolution: $10.4340 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 29.6^\circ$
$T = 298(2) \text{ K}$	$\theta_{\text{min}} = 2.3^\circ$
Rotation method data acquisition using $\omega$ and $\phi$ scans	$h = -9 \rightarrow 9$
Absorption correction: analytical (Clark & Reid, 1995)	$k = -9 \rightarrow 9$
$T_{\text{min}} = 0.943$ , $T_{\text{max}} = 0.993$	$l = -24 \rightarrow 24$
35953 measured reflections	

### Refinement

Refinement on $F^2$	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0618P)^2 + 0.1705P]$
	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.042$	$(\Delta/\sigma)_{\text{max}} < 0.001$

$wR(F^2) = 0.120$

$S = 1.03$

1409 reflections

128 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$\Delta\rho_{\max} = 0.14 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.15 \text{ e } \text{\AA}^{-3}$

Extinction correction: SHELXL97,  
 $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.021 (5)

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C2	1.4392 (4)	0.3530 (4)	0.82976 (16)	0.0655 (7)
H2	1.5569	0.2958	0.8186	0.079*
C3	1.2944 (4)	0.2720 (3)	0.86888 (14)	0.0592 (6)
H3	1.2938	0.1531	0.8890	0.071*
C4	0.9445 (3)	0.3977 (3)	0.90620 (12)	0.0491 (5)
H4A	0.8649	0.3109	0.8781	0.059*
H4B	0.9515	0.3557	0.9581	0.059*
C6	0.7399 (4)	0.6480 (4)	0.95687 (13)	0.0611 (7)
C7	0.6811 (5)	0.8412 (4)	0.93494 (16)	0.0798 (9)
H7A	0.7059	0.9271	0.9759	0.096*
H7B	0.5439	0.8457	0.9224	0.096*
C8	0.8023 (4)	0.8888 (3)	0.86777 (14)	0.0644 (7)
H8A	0.9054	0.9738	0.8817	0.077*
H8B	0.7231	0.9461	0.8290	0.077*
C9	1.0983 (4)	0.7184 (3)	0.81577 (11)	0.0492 (5)
C10	1.1434 (3)	0.4052 (3)	0.87314 (11)	0.0438 (5)
C11	1.2078 (3)	0.5567 (3)	0.83589 (11)	0.0453 (5)
C12	0.8871 (3)	0.7060 (3)	0.83954 (11)	0.0441 (5)
H12	0.8097	0.6622	0.7967	0.053*
N5	0.8583 (3)	0.5804 (2)	0.90326 (9)	0.0456 (4)
O1	1.3924 (2)	0.5282 (3)	0.80864 (9)	0.0597 (5)
O2	1.1586 (3)	0.8488 (3)	0.77918 (11)	0.0746 (6)
O3	0.6908 (3)	0.5644 (4)	1.01363 (11)	0.0947 (8)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C2	0.0502 (12)	0.0705 (16)	0.0759 (16)	0.0132 (12)	-0.0061 (12)	-0.0105 (14)
C3	0.0586 (14)	0.0518 (12)	0.0672 (13)	0.0101 (11)	-0.0137 (12)	-0.0030 (11)
C4	0.0516 (11)	0.0418 (10)	0.0541 (11)	-0.0032 (9)	0.0020 (10)	0.0062 (9)
C6	0.0565 (13)	0.0784 (16)	0.0484 (11)	0.0122 (13)	0.0075 (11)	0.0048 (11)
C7	0.081 (2)	0.0815 (19)	0.0646 (15)	0.0381 (19)	0.0129 (14)	-0.0037 (14)
C8	0.0811 (17)	0.0496 (12)	0.0625 (13)	0.0199 (13)	0.0040 (14)	-0.0008 (11)
C9	0.0604 (13)	0.0456 (11)	0.0415 (9)	-0.0035 (10)	0.0061 (10)	0.0043 (8)

## supplementary materials

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C10	0.0481 (10)	0.0413 (9)	0.0420 (9)	0.0004 (9)	-0.0081 (8)	-0.0026 (8)
C11	0.0440 (10)	0.0484 (11)	0.0436 (9)	-0.0031 (9)	0.0023 (9)	-0.0021 (9)
C12	0.0544 (11)	0.0406 (10)	0.0372 (8)	0.0033 (9)	-0.0016 (9)	0.0013 (8)
N5	0.0492 (9)	0.0447 (9)	0.0430 (8)	0.0020 (8)	0.0062 (8)	0.0037 (7)
O1	0.0457 (9)	0.0710 (11)	0.0623 (9)	-0.0015 (8)	0.0059 (7)	0.0000 (8)
O2	0.0819 (13)	0.0620 (10)	0.0798 (11)	-0.0041 (11)	0.0174 (11)	0.0295 (9)
O3	0.0900 (15)	0.1256 (19)	0.0685 (11)	0.0293 (15)	0.0361 (11)	0.0327 (13)

### *Geometric parameters (Å, °)*

C2—C3	1.347 (4)	C7—H7A	0.9700
C2—O1	1.358 (3)	C7—H7B	0.9700
C2—H2	0.9300	C8—C12	1.527 (3)
C3—C10	1.417 (3)	C8—H8A	0.9700
C3—H3	0.9300	C8—H8B	0.9700
C4—N5	1.447 (3)	C9—O2	1.216 (3)
C4—C10	1.489 (3)	C9—C11	1.434 (3)
C4—H4A	0.9700	C9—C12	1.515 (3)
C4—H4B	0.9700	C10—C11	1.353 (3)
C6—O3	1.221 (3)	C11—O1	1.374 (3)
C6—N5	1.343 (3)	C12—N5	1.462 (2)
C6—C7	1.504 (4)	C12—H12	0.9800
C7—C8	1.493 (4)		
C3—C2—O1	111.8 (2)	C12—C8—H8A	110.5
C3—C2—H2	124.1	C7—C8—H8B	110.5
O1—C2—H2	124.1	C12—C8—H8B	110.5
C2—C3—C10	106.0 (2)	H8A—C8—H8B	108.7
C2—C3—H3	127.0	O2—C9—C11	125.7 (2)
C10—C3—H3	127.0	O2—C9—C12	121.4 (2)
N5—C4—C10	109.22 (17)	C11—C9—C12	112.72 (18)
N5—C4—H4A	109.8	C11—C10—C3	106.4 (2)
C10—C4—H4A	109.8	C11—C10—C4	121.50 (19)
N5—C4—H4B	109.8	C3—C10—C4	132.0 (2)
C10—C4—H4B	109.8	O1—C11—C10	110.68 (19)
H4A—C4—H4B	108.3	O1—C11—C9	121.3 (2)
O3—C6—N5	124.9 (3)	C10—C11—C9	127.4 (2)
O3—C6—C7	126.7 (3)	N5—C12—C9	112.43 (17)
N5—C6—C7	108.5 (2)	N5—C12—C8	103.35 (16)
C6—C7—C8	105.6 (2)	C9—C12—C8	114.0 (2)
C6—C7—H7A	110.6	N5—C12—H12	109.0
C8—C7—H7A	110.6	C9—C12—H12	109.0
C6—C7—H7B	110.6	C8—C12—H12	109.0
C8—C7—H7B	110.6	C6—N5—C12	113.81 (19)
H7A—C7—H7B	108.7	C6—N5—C4	123.63 (19)
C7—C8—C12	106.0 (2)	C12—N5—C4	122.52 (16)
C7—C8—H8A	110.5	C11—O1—C2	105.18 (19)
O1—C2—C3—C10	0.0 (3)	O2—C9—C12—C8	-42.4 (3)
O3—C6—C7—C8	171.7 (3)	C11—C9—C12—C8	142.1 (2)
N5—C6—C7—C8	-8.0 (3)	C7—C8—C12—N5	-16.2 (3)

C6—C7—C8—C12	15.0 (3)	C7—C8—C12—C9	-138.5 (2)
C2—C3—C10—C11	0.3 (3)	O3—C6—N5—C12	177.5 (3)
C2—C3—C10—C4	177.5 (2)	C7—C6—N5—C12	-2.8 (3)
N5—C4—C10—C11	-10.1 (3)	O3—C6—N5—C4	-0.3 (4)
N5—C4—C10—C3	173.0 (2)	C7—C6—N5—C4	179.4 (2)
C3—C10—C11—O1	-0.5 (2)	C9—C12—N5—C6	135.4 (2)
C4—C10—C11—O1	-178.05 (17)	C8—C12—N5—C6	12.1 (3)
C3—C10—C11—C9	170.8 (2)	C9—C12—N5—C4	-46.8 (3)
C4—C10—C11—C9	-6.8 (3)	C8—C12—N5—C4	-170.1 (2)
O2—C9—C11—O1	-6.0 (4)	C10—C4—N5—C6	-144.5 (2)
C12—C9—C11—O1	169.21 (18)	C10—C4—N5—C12	37.9 (3)
O2—C9—C11—C10	-176.4 (2)	C10—C11—O1—C2	0.5 (2)
C12—C9—C11—C10	-1.2 (3)	C9—C11—O1—C2	-171.4 (2)
O2—C9—C12—N5	-159.6 (2)	C3—C2—O1—C11	-0.3 (3)
C11—C9—C12—N5	25.0 (2)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3 $\cdots$ O3 <sup>i</sup>	0.93	2.44	3.278 (3)	150
C2—H2 $\cdots$ O2 <sup>ii</sup>	0.93	2.64	3.374 (3)	136
C12—H12 $\cdots$ O2 <sup>iii</sup>	0.98	2.64	3.344 (3)	129
C8—H8B $\cdots$ O1 <sup>iv</sup>	0.97	2.63	3.547 (3)	157
C8—H8A $\cdots$ O3 <sup>v</sup>	0.97	2.72	3.417 (4)	130

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



Fig. 1

