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## Key indicators

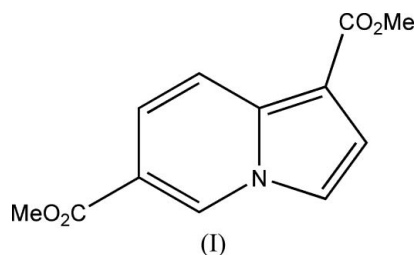
Single-crystal X-ray study  
*T* = 100 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$   
*R* factor = 0.043  
*wR* factor = 0.115  
Data-to-parameter ratio = 19.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## Dimethyl indolizine-1,6-dicarboxylate

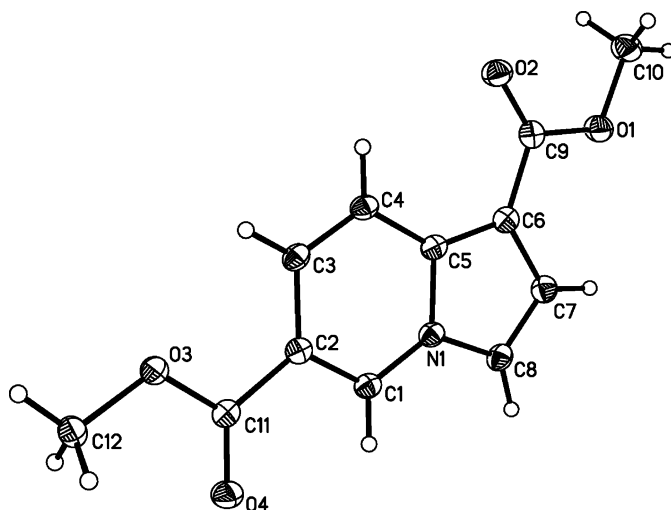
In the title compound,  $\text{C}_{11}\text{H}_{11}\text{NO}_4$ , the indolizine unit is almost planar. The two carboxylate groups are coplanar with the indolizine moiety. The packing is stabilized by intermolecular  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonds.

## Comment

Indolizines are electron-rich heterocycles. 3-Unsubstituted indolizine is especially important in the family of indolizines, as the highest electronic population in the  $\pi$ -excessive heterocycle focuses on C3, which allows many electrophilic substitutions (Reid *et al.*, 1979).



The structure of the title compound, (I), has been determined as we use 3-unsubstituted indolizines as electrophilic substituted reagents. The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987), and comparable with those in related structures (Usman *et al.*, 2002). In the title structure (Fig. 1), all C atoms are almost planar, the torsion angles around the indolizine unit ranging from 0.11 (12) to



**Figure 1**  
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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1.59 (7)°. The carboxylate groups are nearly coplanar with the indolizine unit. Coplanarity is influenced by an intramolecular C9—H9···O2 hydrogen bond.

The crystal structure of (I) exhibits hydrogen-bond interactions (Table 1); these help to stabilize the crystal structure (Fig. 2).

## Experimental

A suspension of 3-(carboxymethyl)pyridinium chloride (10 mmol) methyl acrylate (50 mmol) and Et<sub>3</sub>N (1.5 ml) in toluene (80 ml) was stirred at 363 K for 2 h (monitored by thin-layer chromatography). The resulting solid was filtered off, and the organic layer was evaporated and chromatographed to give (I) (yield 56%; m.p. 423–424 K) (Zhang *et al.*, 2000). Single crystals suitable for X-ray crystallographic analysis were obtained by recrystallization from a petroleum ether–acetone solution (3:1 v/v).

### Crystal data

C <sub>12</sub> H <sub>11</sub> NO <sub>4</sub>	Z = 4
M <sub>r</sub> = 233.22	D <sub>x</sub> = 1.486 Mg m <sup>-3</sup>
Monoclinic, P2 <sub>1</sub> /c	Mo Kα radiation
a = 14.3617 (3) Å	μ = 0.11 mm <sup>-1</sup>
b = 3.83580 (10) Å	T = 100.0 (1) K
c = 19.4547 (3) Å	Block, yellow
β = 103.3550 (10)°	0.52 × 0.21 × 0.12 mm
V = 1042.75 (4) Å <sup>3</sup>	

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	13030 measured reflections
φ and ω scans	3041 independent reflections
Absorption correction: multi-scan (XCAD4; Harms & Wocadlo 1995)	2516 reflections with I > 2σ(I)
T <sub>min</sub> = 0.944, T <sub>max</sub> = 0.986	R <sub>int</sub> = 0.029
	θ <sub>max</sub> = 30.0°

### Refinement

Refinement on F <sup>2</sup>	w = 1/[σ <sup>2</sup> (F <sub>o</sub> <sup>2</sup> ) + (0.0556P) <sup>2</sup> + 0.3698P]
R[F <sup>2</sup> > 2σ(F <sup>2</sup> )] = 0.043	where P = (F <sub>o</sub> <sup>2</sup> + 2F <sub>c</sub> <sup>2</sup> )/3
wR(F <sup>2</sup> ) = 0.115	(Δ/σ) <sub>max</sub> = 0.001
S = 1.07	Δρ <sub>max</sub> = 0.41 e Å <sup>-3</sup>
3041 reflections	Δρ <sub>min</sub> = -0.21 e Å <sup>-3</sup>
156 parameters	
H-atom parameters constrained	

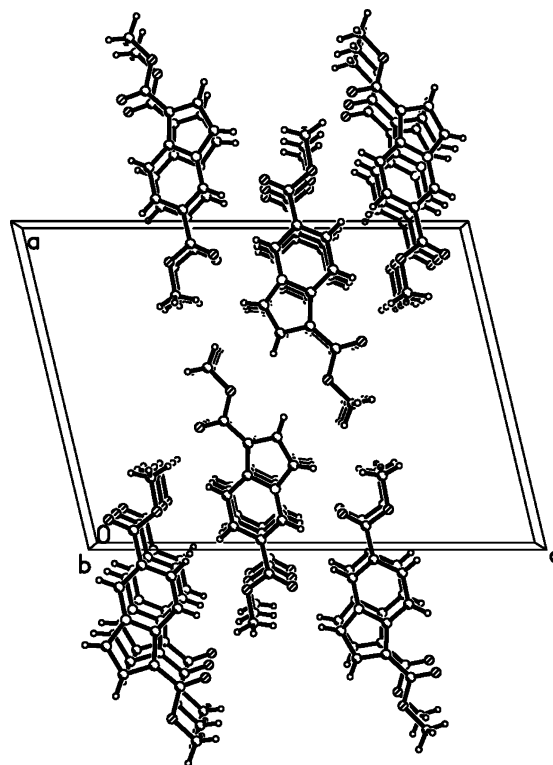
**Table 1**

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O4 <sup>i</sup>	0.93	2.43	3.237 (2)	144
C12—H12A···O2	0.96	2.47	2.406 (6)	164

Symmetry code: (i) -x + 2, -y + 2, -z.

H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances in the range 0.93–0.97 Å, and with U<sub>iso</sub>(H) = 1.2U<sub>eq</sub>(parent atom), or U<sub>iso</sub>(H) = 1.5U<sub>eq</sub>(C<sub>methyl</sub>).



**Figure 2**

The packing of the molecule of (I), viewed along the b axis.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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