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Methyl pyrrolo[2,1-*a*]isoquinoline-1-carboxylate

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Key indicators

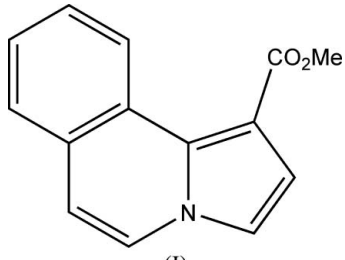
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.001 Å
R factor = 0.047
wR factor = 0.129
Data-to-parameter ratio = 36.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{14}H_{11}NO_2$, the indolizine unit is almost planar. The carboxylate group is oriented almost coplanar with the indolizine unit.

Comment

Indolizines are electron-rich heterocycles. 3-Unsubstituted indolizine is especially important in the family of indolizines, since the highest electron population occurs on C3, which allows many electrophilic substitutions (Reid *et al.*, 1979). The structure of the title compound, (I), was obtained when we used 3-unsubstituted indolizine as an electrophilic substitution reagent.



(I)

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), the indolizine unit is completely planar and almost coplanar with the the carboxylate group, with a dihedral angle between the aromatic rings and the carboxylate group of 7.38 (4)°. No classical hydrogen bonds were found.

Experimental

A suspension of 2-(carboxymethyl)isoquinolinium bromide (10 mmol), methyl acrylate (50 mmol) and Et_3N (1.5 ml) in toluene (80 ml) was stirred at 363 K for 2 h (monitored by thin-layer chromatography). The solid was filtered off and the organic layer was evaporated and chromatographed to give (I) in a yield of 83% (Zhang *et al.*, 2000). Single crystals suitable for X-ray crystallographic analysis were obtained by recrystallization from acetone and petroleum ether (1:3 *v*/*v*).

Crystal data

$C_{14}H_{11}NO_2$
M_r = 225.24
Monoclinic, $P2_1/c$
a = 9.8733 (1) Å
b = 6.9155 (1) Å
c = 15.7532 (2) Å
β = 97.283 (1)°
V = 1066.93 (2) Å^3
Z = 4
D_x = 1.402 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100.0 (1) K
Block, colorless
0.48 × 0.35 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (SABADS; Bruker, 2005)
T_{min} = 0.956, T_{max} = 0.978
49755 measured reflections
5583 independent reflections
4751 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 37.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.129
S = 1.00
5583 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 0.2336P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C3	1.3847 (9)	C12—C13	1.4596 (9)
C3—N1—C11	124.21 (6)	C9—C10—C11	123.11 (6)
C2—N1—C3—C4	178.83 (7)	C10—C11—C12—C13	2.10 (14)
C11—N1—C3—C4	−0.41 (11)		

H atoms were positioned geometrically and refined as riding on their parent C atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

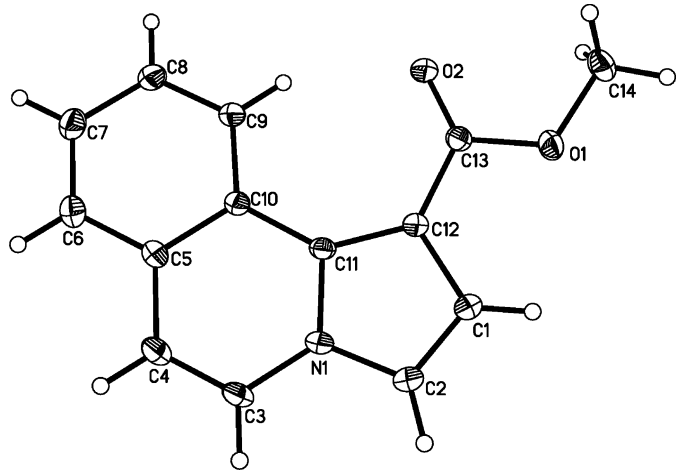


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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