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Dimethyl 7-(*N*,*N*-dimethylamino)-3-(2-methoxybenzoyl)indolizine-1,2-dicarboxylate

R. Hema,[a] V. Parthasarathi,[a]* K. Ravikumar,[b] K. Sarkunam[c] and M. Nallu[c]

[a]Department of Physics, Bharathidasan University, Tiruchirappalli 620 024, India, [b]Laboratory of X-ray Crystallography, Indian Institute of Chemical Technology, Hyderabad 500 007, India, and [c]Department of Chemistry, Bharathidasan University, Tiruchirappalli 620 024, India

Correspondence e-mail: vpsarati@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.060
wR factor = 0.147
Data-to-parameter ratio = 12.6

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

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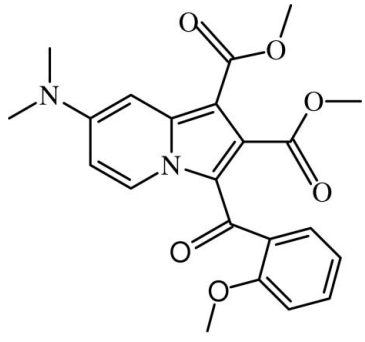
In the title molecule, $C_{22}H_{22}N_2O_6$, the planes of the two methoxycarbonyl groups are oriented at angles of 5.19 (14) and 80.21 (9)° with respect to that of the indolizine ring. In the crystal structure, the molecules are linked by weak intermolecular C—H···O interactions to form centrosymmetric ring motifs.

Comment

Heterocyclic compounds such as indolizines are important bioactive compounds that have a wide range of applications in biology, pharmacology and agrochemistry (Wu & Chen, 2003). Indolizines have also been tested as antimycobacterial agents against mycobacterial tuberculosis (Gundersen *et al.*, 2003). Due to the diverse properties of indolizine derivatives, the structure of the title compound, (I), has been determined as part of our study on the conformational changes caused by different substituents at various positions on the indolizine ring system.



(I)

The bond lengths and bond angles in (I) are comparable with those in related structures (Hema *et al.*, 2003, 2004). The non-H atoms of (I) common to two related indolizine derivatives, dimethyl 3-benzoyl-7-(*N*,*N*-dimethylamino)indolizine-1,2-dicarboxylate and 3-(4-bromobenzoyl)-7-(*N*,*N*-dimethylamino)indolizine-1,2-dicarboxylate (Hema *et al.*, 2003, 2004), were superimposed on the corresponding atoms of these latter compounds and the r.m.s. deviations were found to be 1.2 and 0.86 Å, respectively. The planes of the two methoxycarbonyl groups deviate from the plane of the indolizine ring to different extents. The angles between the indolizine plane and that of the C1/C10/O10/O11/C12 and C2/C13/O13/O14/C15 groups are 5.19 (14) and 80.21 (9)°, respectively. The dihedral angle between the planes of the methoxyphenyl ring and the indolizine ring system is 85.96 (7)°, while the plane of the carbonyl group C3/C16/O16/C17 makes angles of 77.06 (10)

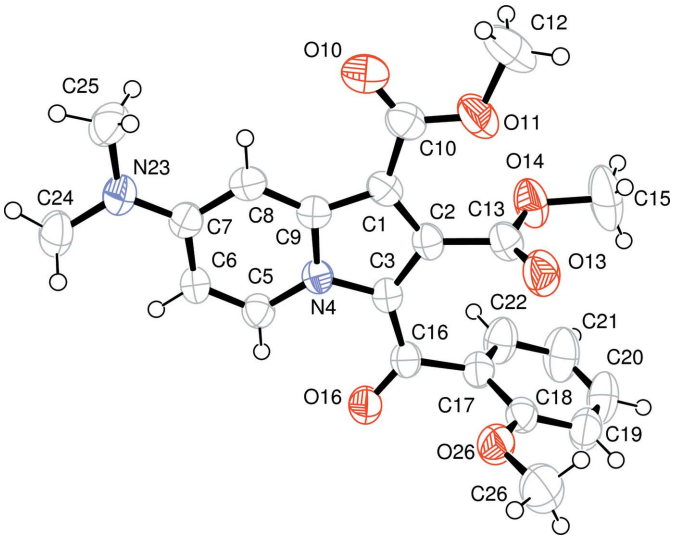


Figure 1
View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.

and 9.95 (12)° with the planes of the methoxyphenyl ring and the indolizine ring system, respectively.

The crystal packing is influenced by weak intermolecular C—H···O interactions and C—H···π interactions (Table 1). The C15—H151···O13 interaction links pairs of molecules related by a centre of inversion, generating an $R_2^2(10)$ motif (Bernstein *et al.*, 1995). Atom C6 (*via* H6) acts as a donor for a weak intermolecular C—H···π interaction with the centroid (*Cg*1) of benzene ring C17–C21 in the molecule at $(\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z)$.

Experimental

A mixture of 4-dimethylaminopyridinium-1-(2-methoxy)phenacylide (1.4 mmol), dimethyl acetylenedicarboxylate (1.6 mmol) and potassium carbonate (1.6 mmol) in dimethylformamide (30 ml) was allowed to stand at room temperature overnight. The insoluble materials were removed by filtration. The filtrate was extracted with an ethyl acetate–dilute HCl mixture (70:30 *v*/*v*). The organic layer was evaporated and chromatographed to give (I), which was recrystallized from ethyl acetate (yield 48%, m.p. 447–449 K).

Crystal data

$C_{22}H_{22}N_2O_6$
M_r = 410.42
Monoclinic, $C2/c$
a = 28.878 (3) Å
b = 8.0015 (8) Å
c = 18.7634 (18) Å
β = 109.547 (2)°
V = 4085.7 (7) Å^3
Z = 8
D_x = 1.334 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2107 reflections
θ = 2.3–24.1°
μ = 0.10 mm^{-1}
T = 293 (2) K
Prism, yellow
0.28 × 0.18 × 0.15 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
10194 measured reflections
3481 independent reflections
2589 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.0°
$h = -34 \rightarrow 34$
$k = -9 \rightarrow 9$
$l = -22 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.147
S = 1.12
3481 reflections
276 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 1.9395P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

*Cg*1 is the centroid of benzene ring C17–C21.

D—H···A	D—H	H···A	D···A	D—H···A
C15—H151···O13^{i}	0.96	2.54	3.486 (5)	169
C6—H6···*Cg*1^{ii}	0.93	2.92	3.742 (3)	149

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

The methyl H atoms were constrained to an ideal geometry (C—H = 0.96 Å), with U_{iso} values of $1.5U_{eq}$(C), but were allowed to rotate freely about the C—C bond. All remaining H atoms were placed in idealized positions (C—H = 0.93 Å) and constrained to ride on their parent atoms, with U_{iso}(H) values of $1.2U_{eq}$(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Version 1.07; Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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