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4-(2,2-Dichloro-*N*-methylacetamido)phenyl furan-2-carboxylate

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Key indicators

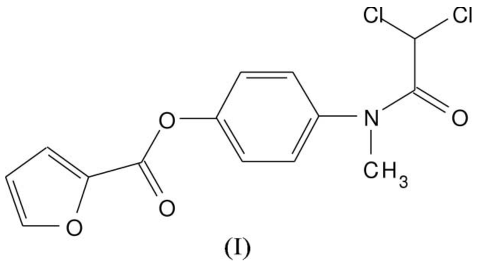
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.143
Data-to-parameter ratio = 13.1

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

In the title compound, $C_{14}H_{11}Cl_2NO_4$, the dihedral angle between the two aromatic rings is 47.39 (13)°. The crystal packing is stabilized by C—H···O hydrogen bonds.

Comment

Amoebiosis is a major public health problem in tropical and subtropical countries (McAuley *et al.*, 1992). Diloxanide furoate, (I), is the mainstay for treating asymptomatic cyst carriers and one of the oldest dichloroacetamide derivative drugs for the treatment of amoebiosis. A crystal structure determination was carried out in order to elucidate the molecular conformation.



(I)

A perspective view of (I) is shown in Fig. 1. In (I), the furan ring is planar. The dihedral angle between the furan ring and the benzene ring is 47.39 (13)°. The keto group is almost coplanar with the furan ring, as indicated by the C1—C2—C6—O7 torsion angle of −8.5 (4)°, and is in a synperiplanar conformation [O7—C6—O8—C9 = 8.3 (3)°]. The other keto group adjacent to the *N*-methyl unit is in an antiperiplanar conformation, as indicated by the C12—N15—C17—O18 torsion angle of 177.9 (2)°. The 2,2-dichloroacetylmethylamino group at the 4 position of the benzene ring is rotated 80.3 (1)° from the plane of the benzene ring. The crystal packing is stabilized by C—H···O hydrogen bonding (Table 1). The molecules form hydrogen-bonded dimers.

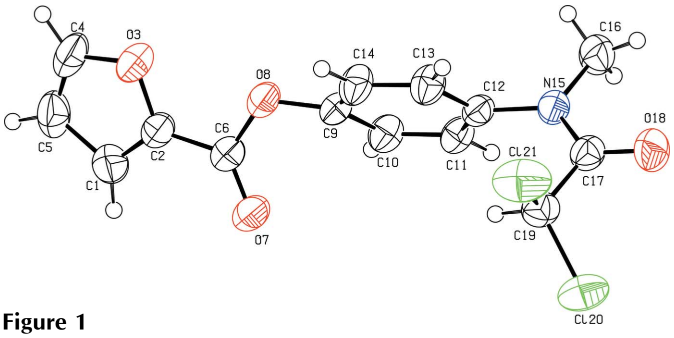


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids.

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Experimental

Diloxanide furoate (1.5 g) was dissolved in methanol (30 ml). Charcoal (3.5 g) was added and the mixture was stirred with heating for 6 minutes on a Deepali Stirrer (MS-4) at 1150 r.p.m. The hot solution was filtered through Whatmann 42 filter paper and kept in a slightly open, stoppered conical flask. Rectangular pale-green crystals grew by thin-film evaporation.

Crystal data

$C_{14}H_{11}Cl_2NO_4$
$M_r = 328.14$
Monoclinic, $P2_1/n$
$a = 8.334\ (5)$ Å
$b = 10.778\ (5)$ Å
$c = 16.412\ (10)$ Å
$\beta = 103.761\ (2)^\circ$
$V = 1431.9\ (14)$ Å^3
$Z = 4$
$D_x = 1.522$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.47$ mm^{-1}
$T = 295\ (2)$ K
Block, pale green
$0.25 \times 0.24 \times 0.22$ mm

Data collection

MacScience DIPLabo 32001 diffractometer
ω scans
Absorption correction: none
4433 measured reflections
2524 independent reflections
2209 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\rm max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.143$
$S = 1.20$
2524 reflections
192 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0816P)^2 + 0.2846P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.35$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.30$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.056 (5)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C4—H4$\cdots$O18$^{\rm i}$	0.93	2.41	3.285 (4)	156

Symmetry code: (i) $x - \frac{3}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$.

H atoms were placed at idealized positions and allowed to ride on their parent atoms, with C—H = 0.92—0.98 Å and N—H = 0.86 Å; $U_{\rm iso}$(H) values were set equal to $xU_{\rm eq}$(carrier atom), where $x = 1.5$ for methyl H atoms and $x = 1.2$ for all other H atoms.

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *PLATON* (Spek, 2003).

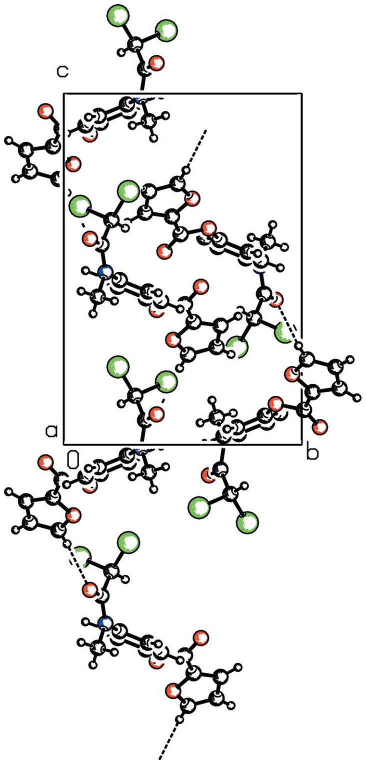

Figure 2
The packing of (I), viewed down the c axis. Dashed lines indicate hydrogen bonds.

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