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(2-Methylphenoxy)acetic acid

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Key indicators

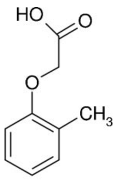
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.078
wR factor = 0.230
Data-to-parameter ratio = 11.3

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

Dimeric hydrogen bonding is present in the crystal structure of (2-methylphenoxy)acetic acid, $C_9H_{10}O_3$, involving the carboxylate groups of centrosymmetrically related pairs of molecules. The structure is further stabilized by C—H···O hydrogen bonding.

Comment

The title compound, (I), also known as (*o*-tolyloxy)acetic acid, has been described as an expectorant (Negwer, 1996), and several phenoxyacetic acid compounds are used as herbicides (Cserhati & Forgacs, 1998).



(I)

The atomic arrangement in (I) is shown in Fig. 1 and selected geometric parameters are given in Table 1. Apart from the H atoms, the molecule is essentially planar and the torsion angle with the greatest deviation from 0, or ±180°, is C2—O1—C7—C8 = 175.6 (2)°.

Carboxylic acids normally form dimers or catemers and here, as expected for a simple monocarboxylic acid, dimers are formed by intermolecular hydrogen bonding involving the carboxylate groups. The pairs of molecules forming the dimers are related by a centre of symmetry and details of the hydrogen bonding are given in Table 2. As well as the dimeric $R_2^2(8)$ motif, a weak C—H···O contact (Table 2) is present and

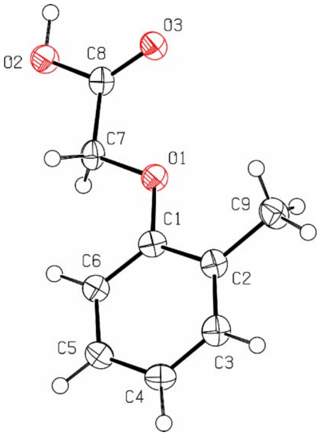


Figure 1
The atomic arrangement in the molecule of (I), with the the atom-numbering scheme and 50% probability displacement ellipsoids.

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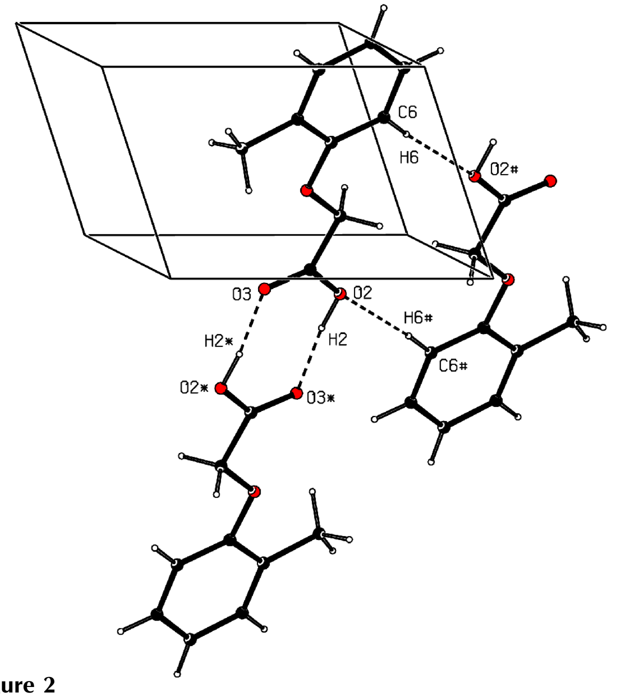

Figure 2
A partial packing diagram of (I), showing $R_2^2(8)$ and $R_2^2(14)$ ring formations. [Symmetry codes: (*) $-1 - x, -y, 1 - z$; (#) $-x, -y, 2 - z$.]

this links two molecules about a centre of symmetry in an $R_2^2(14)$ formation (Fig. 2). Hence, atom O2 acts as both a donor and an acceptor. Indications of C—H$\cdots\pi$ bonding (Table 2) are also present as H7*A* is close to the centroid (*Cg*1) of the aromatic ring.

There are many similar examples of dimer formation involving carboxylate groups *e.g.* phenylacetic acid (Hodgson & Asplund, 1991) and 2,4,5-trimethylbenzoic acid (Barcon *et al.*, 1997). The solid-state structures of related compounds, *viz.* (4-methylphenoxy)acetic acid (Kumar & Rao, 1982) and 3-(2-hydroxyphenyl)propionic acid (Begum *et al.*, 1992), have also been determined.

Experimental

The title compound was obtained from Aldrich and was recrystallized from a mixture of methanol and ethanol.

Crystal data

$C_9H_{10}O_3$
$M_r = 166.17$
Monoclinic, $P2_1/c$
$a = 5.1062$ (5) Å
$b = 22.352$ (2) Å
$c = 7.4014$ (9) Å
$\beta = 108.235$ (5)°
$V = 802.33$ (14) Å^3
$Z = 4$
$D_x = 1.376$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2909 reflections
$\theta = 3.0$–27.5°
$\mu = 0.10$ mm^{-1}
$T = 150$ (2) K
Plate, colourless
0.40 × 0.24 × 0.06 mm

Data collection

Enraf–Nonius KappaCCD area detector
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{\min} = 0.97$, $T_{\max} = 0.99$
2908 measured reflections
1304 independent reflections
1006 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.055$
$\theta_{\max} = 27.5°$
$h = -6 \rightarrow 5$
$k = -28 \rightarrow 29$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.078$
$wR(F^2) = 0.230$
$S = 1.04$
1304 reflections
115 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1765P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.36$ e Å^{-3}
$\Delta\rho_{\min} = -0.53$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.07 (2)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.381 (3)	O2—C8	1.322 (3)
O1—C7	1.415 (3)	O3—C8	1.219 (3)
C1—O1—C7	116.32 (19)	O3—C8—C7	124.8 (2)
O1—C1—C2	114.7 (2)	O2—C8—C7	110.8 (2)
O3—C8—O2	124.4 (2)		
O1—C1—C2—C9	3.7 (4)	C1—O1—C7—C8	175.6 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O2—H2$\cdots$O3$^{\rm i}$	0.93 (4)	1.69 (4)	2.618 (3)	172 (4)
C6—H6$\cdots$O2$^{\rm ii}$	0.95	2.56	3.505 (3)	175
C7—H7*A*$\cdots$*Cg*1$^{\rm iii}$	0.99	2.60	3.37	134

Symmetry codes: (i) $-1 - x, -y, 1 - z$; (ii) $-x, -y, 2 - z$; (iii) $x - 1, y, z$. *Cg*1 is the centroid of the aromatic ring.

The crystal diffracted very weakly and decomposed during data collection, hence data completeness is only 71%. The hydroxy (O2) H atom was refined isotropically. The C—H H atoms were allowed to ride on their attached C atoms: C—H distances were 0.95 Å (aromatic), 0.99 Å (methylene) and 0.98 Å (methyl), and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(non-methyl C) or $1.4U_{\rm eq}$(methyl C).

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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