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(2,3-Dimethylphenoxy)acetic acid

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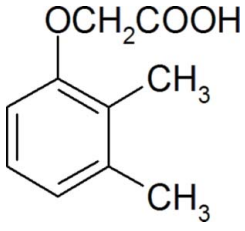
Key indicators: single-crystal X-ray study; T = 103 K; mean σ(C–C) = 0.001 Å; R factor = 0.040; wR factor = 0.119; data-to-parameter ratio = 20.4.

The acetic acid substituent of the title compound, $C_{10}H_{12}O_3$, is coplanar with the 2,3-dimethylphenoxy group. The crystal structure is stabilized by intermolecular hydrogen-bond interactions.

Related literature

For related structures, see: Chandrasekhar & Pattabhi (1977); Kumar & Rao (1980, 1982); Smith *et al.* (1981, 1986); Kennard & Smith (1981); Kennard *et al.* (1981, 1982); Hegde *et al.* (1991); Cox & Hickey (2004); Byres & Cox (2007). For background, see: Cremlyn (1978); Gruzdyev *et al.* (1983); Elliott (2005). For synthesis, see: Vogel (1989).



Experimental

Crystal data

$C_{10}H_{12}O_3$
M_r = 180.20
Triclinic, $P\overline{1}$
a = 6.7609 (6) Å
b = 6.8452 (6) Å
c = 10.783 (1) Å
α = 72.549 (1)°
β = 81.202 (1)°
γ = 67.756 (1)°
V = 440.20 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 103 K
0.76 × 0.58 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*DENZO/SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.928, T_{max} = 0.969
4991 measured reflections
2463 independent reflections
2321 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.119
S = 1.03
2463 reflections
121 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O3^{i}	0.84	1.79	2.6269 (9)	172

Symmetry code: (i) $-x+2, -y+1, -z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2090).

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supplementary materials

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(2,3-Dimethylphenoxy)acetic acid

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Comment

Phenoxyacetic acids are well known herbicides. It is also known that indole-3-acetic acid promotes cell elongation in plants and was isolated from plants and this stimulated the search for other compounds of related structure. This created great interest in aryloxyacetic acids as potential plant growth regulators and large number of phenoxyacetic acids are used as herbicides. Phenoxyacetic acid is used as a precursor in antibiotic fermentations especially for penicillin V and is a main skeleton of plant growth regulators and herbicides. It is used as an intermediate for manufacturing dyes, pharmaceuticals, pesticides, fungicides. It is used in flavoring. A review on the genotoxicity of 4-chloro-2-methylphenoxyacetic acid is described. In view of the importance of the title compound, (I), $C_{10}H_{12}O_3$, the crystal structure is reported.

The acetic acid ligand of the title compound is in the plane of the 2,3-dimethylphenoxy group with a C7—O1—C1—C2 torsion angle of −178.60 (6)°.

Experimental

Title aryloxy acetic acid, $C_{10}H_{12}O_3$, (I), was prepared according to the literature method (Vogel, 1989) and was crystallized from acetone by slow evaporation (m.p.: 360 K).

Refinement

All of the H atoms, except H2 which was located from difference Fourier map, were inferred from neighbouring sites. All H-atoms were included in the riding model approximation with C—H = 0.95–0.99 Å, and with U_{iso}(H) = 1.18–1.51U_{eq}(C).

Figures

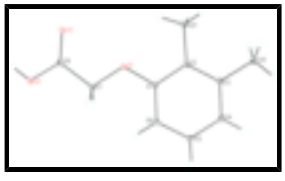

Fig. 1. Molecular structure of $C_{10}H_{12}O_3$, (I), showing atom labeling and 50% probability displacement ellipsoids.

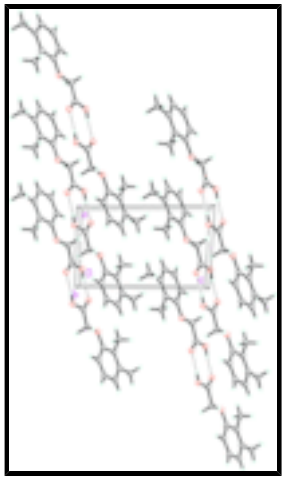

Fig. 2. Packing diagram of $C_{10}H_{12}O_3$viewed down the *b* axis. Dashed lines indicate C—H···O hydrogen bonds between O2—H2 and O3 from inverted, in-plane adjacent molecules in the title compound.

(2,3-Dimethylphenoxy)acetic acid

Crystal data

$C_{10}H_{12}O_3$	$Z = 2$
$M_r = 180.20$	$F_{000} = 192$
Triclinic, $P\overline{1}$	$D_x = 1.359$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.7609$ (6) Å	Cell parameters from 4023 reflections
$b = 6.8452$ (6) Å	$\theta = 0.00$–0.00^o
$c = 10.783$ (1) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 72.549$ (1)°	$T = 103$ K
$\beta = 81.202$ (1)°	Prism, colorless
$\gamma = 67.756$ (1)°	0.76 × 0.58 × 0.32 mm
$V = 440.20$ (7) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2463 independent reflections
Radiation source: fine-focus sealed tube	2321 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.015$
$T = 103$ K	$\theta_{max} = 30.7^o$
φ and ω scans	$\theta_{min} = 2.0^o$
Absorption correction: multi-scan (DENZO/SCALEPACK; Otwinowski & Minor, 1997)	$h = -9 \rightarrow 9$
$T_{min} = 0.928$, $T_{max} = 0.969$	$k = -9 \rightarrow 7$
4991 measured reflections	$l = -14 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H-atom parameters constrained
$wR(F^2) = 0.119$	$w = 1/[\sigma^2(F_o^2) + (0.0769P)^2 + 0.1045P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.013$
2463 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
121 parameters	$\Delta\rho_{min} = -0.36$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.40060 (9)	0.53274 (10)	0.17282 (6)	0.01580 (15)
O2	0.77872 (10)	0.74592 (10)	−0.02470 (6)	0.01806 (16)
H2	0.9099	0.6872	−0.0414	0.022*
O3	0.81153 (9)	0.40211 (10)	0.08982 (6)	0.01629 (16)
C1	0.19165 (12)	0.60157 (13)	0.22166 (8)	0.01308 (17)
C2	0.12308 (12)	0.43570 (13)	0.30554 (8)	0.01355 (17)
C21	0.27567 (14)	0.20182 (14)	0.33949 (9)	0.01978 (19)
H21A	0.2670	0.1386	0.4337	0.030*
H21B	0.4219	0.1979	0.3123	0.030*
H21C	0.2373	0.1170	0.2946	0.030*
C3	−0.08874 (13)	0.49346 (13)	0.35611 (8)	0.01427 (17)
C31	−0.17245 (14)	0.31989 (15)	0.44193 (9)	0.01932 (19)
H31A	−0.3247	0.3876	0.4639	0.029*
H31B	−0.0932	0.2491	0.5219	0.029*
H31C	−0.1538	0.2103	0.3957	0.029*
C4	−0.22446 (13)	0.71328 (14)	0.32598 (8)	0.01596 (18)
H4A	−0.3672	0.7520	0.3616	0.019*
C5	−0.15242 (13)	0.87504 (13)	0.24465 (8)	0.01634 (18)

H5A	−0.2455	1.0236	0.2257	0.020*
C6	0.05604 (13)	0.82050 (13)	0.19054 (8)	0.01513 (17)
H6A	0.1049	0.9304	0.1335	0.018*
C7	0.47291 (12)	0.69872 (13)	0.09072 (8)	0.01408 (17)
H7A	0.4546	0.8102	0.1367	0.017*
H7B	0.3879	0.7715	0.0119	0.017*
C8	0.70550 (12)	0.59811 (13)	0.05272 (8)	0.01343 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0109 (3)	0.0134 (3)	0.0199 (3)	−0.0050 (2)	0.0046 (2)	−0.0017 (2)
O2	0.0144 (3)	0.0151 (3)	0.0233 (3)	−0.0077 (2)	0.0051 (2)	−0.0028 (2)
O3	0.0143 (3)	0.0143 (3)	0.0191 (3)	−0.0060 (2)	0.0017 (2)	−0.0027 (2)
C1	0.0110 (3)	0.0136 (4)	0.0142 (3)	−0.0048 (3)	0.0019 (3)	−0.0038 (3)
C2	0.0127 (3)	0.0131 (3)	0.0142 (3)	−0.0050 (3)	0.0018 (3)	−0.0032 (3)
C21	0.0184 (4)	0.0130 (4)	0.0222 (4)	−0.0033 (3)	0.0044 (3)	−0.0021 (3)
C3	0.0137 (3)	0.0161 (4)	0.0136 (3)	−0.0071 (3)	0.0022 (3)	−0.0038 (3)
C31	0.0177 (4)	0.0185 (4)	0.0214 (4)	−0.0099 (3)	0.0056 (3)	−0.0034 (3)
C4	0.0121 (3)	0.0176 (4)	0.0169 (4)	−0.0045 (3)	0.0023 (3)	−0.0051 (3)
C5	0.0140 (4)	0.0140 (4)	0.0181 (4)	−0.0028 (3)	0.0006 (3)	−0.0036 (3)
C6	0.0142 (3)	0.0131 (4)	0.0167 (4)	−0.0054 (3)	0.0015 (3)	−0.0022 (3)
C7	0.0118 (3)	0.0131 (3)	0.0166 (4)	−0.0060 (3)	0.0023 (3)	−0.0025 (3)
C8	0.0129 (3)	0.0152 (4)	0.0138 (3)	−0.0069 (3)	0.0012 (3)	−0.0047 (3)

Geometric parameters (Å, °)

O1—C1	1.3829 (9)	C3—C31	1.5092 (11)
O1—C7	1.4136 (9)	C31—H31A	0.9800
O2—C8	1.3084 (10)	C31—H31B	0.9800
O2—H2	0.8400	C31—H31C	0.9800
O3—C8	1.2295 (10)	C4—C5	1.3884 (11)
C1—C6	1.3969 (11)	C4—H4A	0.9500
C1—C2	1.4059 (11)	C5—C6	1.3953 (11)
C2—C3	1.4022 (11)	C5—H5A	0.9500
C2—C21	1.5083 (11)	C6—H6A	0.9500
C21—H21A	0.9800	C7—C8	1.5057 (11)
C21—H21B	0.9800	C7—H7A	0.9900
C21—H21C	0.9800	C7—H7B	0.9900
C3—C4	1.4015 (11)		
C1—O1—C7	116.00 (6)	H31A—C31—H31C	109.5
C8—O2—H2	109.5	H31B—C31—H31C	109.5
O1—C1—C6	122.84 (7)	C5—C4—C3	120.66 (7)
O1—C1—C2	115.49 (7)	C5—C4—H4A	119.7
C6—C1—C2	121.68 (7)	C3—C4—H4A	119.7
C3—C2—C1	118.45 (7)	C4—C5—C6	120.34 (7)
C3—C2—C21	121.37 (7)	C4—C5—H5A	119.8
C1—C2—C21	120.18 (7)	C6—C5—H5A	119.8

C2—C21—H21A	109.5	C5—C6—C1	118.89 (7)
C2—C21—H21B	109.5	C5—C6—H6A	120.6
H21A—C21—H21B	109.5	C1—C6—H6A	120.6
C2—C21—H21C	109.5	O1—C7—C8	109.13 (6)
H21A—C21—H21C	109.5	O1—C7—H7A	109.9
H21B—C21—H21C	109.5	C8—C7—H7A	109.9
C4—C3—C2	119.94 (7)	O1—C7—H7B	109.9
C4—C3—C31	119.68 (7)	C8—C7—H7B	109.9
C2—C3—C31	120.38 (7)	H7A—C7—H7B	108.3
C3—C31—H31A	109.5	O3—C8—O2	124.77 (7)
C3—C31—H31B	109.5	O3—C8—C7	124.00 (7)
H31A—C31—H31B	109.5	O2—C8—C7	111.23 (7)
C3—C31—H31C	109.5		
C7—O1—C1—C6	1.44 (12)	C2—C3—C4—C5	1.00 (12)
C7—O1—C1—C2	−178.60 (6)	C31—C3—C4—C5	−178.41 (7)
O1—C1—C2—C3	−178.50 (7)	C3—C4—C5—C6	0.67 (13)
C6—C1—C2—C3	1.46 (12)	C4—C5—C6—C1	−1.25 (13)
O1—C1—C2—C21	1.53 (12)	O1—C1—C6—C5	−179.87 (7)
C6—C1—C2—C21	−178.51 (7)	C2—C1—C6—C5	0.18 (13)
C1—C2—C3—C4	−2.03 (12)	C1—O1—C7—C8	176.74 (6)
C21—C2—C3—C4	177.94 (7)	O1—C7—C8—O3	−0.52 (11)
C1—C2—C3—C31	177.38 (7)	O1—C7—C8—O2	179.29 (6)
C21—C2—C3—C31	−2.65 (12)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O3^{i}	0.84	1.79	2.6269 (9)	172

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*.

Fig. 1

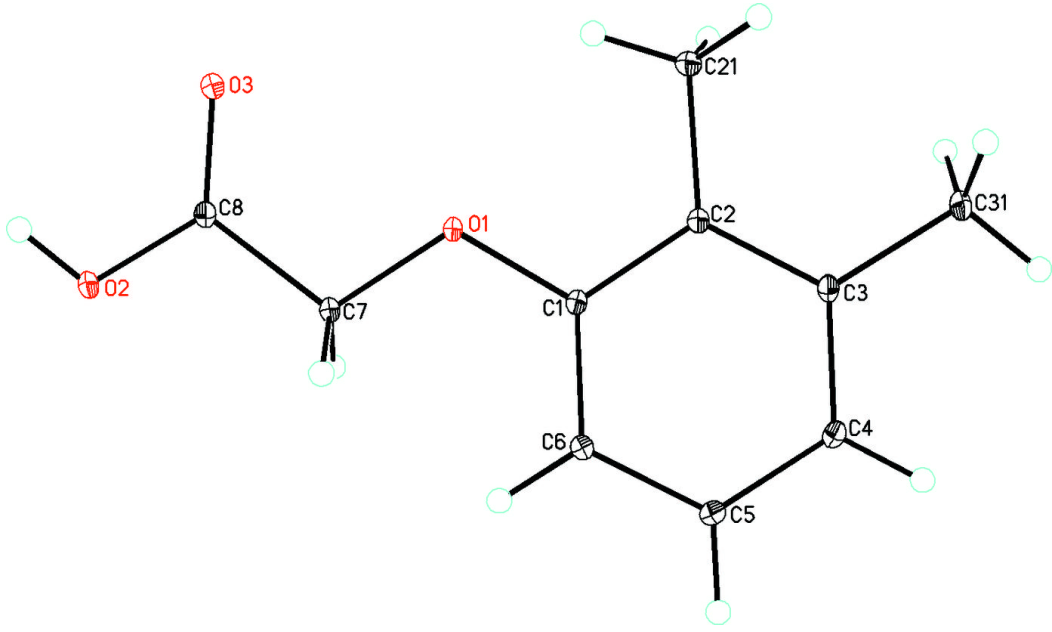

Fig. 2