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Methyl 3-(4-hydroxyphenyl)propionate

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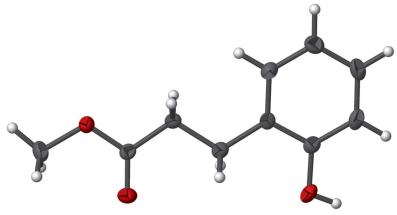
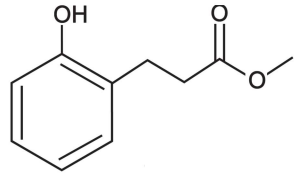
The title compound, $C_{10}H_{12}O_3$, crystallizes in the orthorhombic $P2_12_12_1$ space group. The structure contains a phenolic group with the OH being coplanar with the phenyl ring. The structure exhibits significant hydrogen bonding between the O—H group of one molecule and the CO group of an adjacent one. These O—H···O=C interactions form chains of molecules parallel to the *b* axis. No π–π or C—H···π intermolecular interactions are observed.

3D view



Chemical scheme



Structure description

The application of nitrogen-based fertilizers has been a remarkable strategy applied to meet the growing world food and fibre demands over the past 80 years (Galloway *et al.*, 2008). However, these fertilizers increase anthropogenic nitrous oxide production, causing serious effects on the environment in water, the air and soil. One of the important environmentally friendly techniques applied in agriculture to control the rate of the climate-relevant N_2O gas emission is the use of nitrification inhibitors (Ruser & Schulz, 2015). Among the various nitrification inhibitors, methyl 3-(2 or 4-hydroxyphenyl)propionates (MHPPs) are the most important formed in sorghum (Sorghum bicolor; Zakir *et al.*, 2008; Nardi *et al.*, 2013). Additionally, they exhibit an interesting motif in the enzymatic coupling of saccharides to proteins, also acting as modulators of the root system architecture (RSA; Martinez *et al.*, 2017; ter Haar *et al.*, 2011). There are various reports on the synthesis of methyl 3-(2-hydroxyphenyl)propionate (Yuthavong *et al.*, 2012; Rosales *et al.*, 2011; Meier *et al.*, 2006), but its crystal structure has not previously been been reported. As part of our ongoing studies on the synthesis and properties of phenolic compounds (Abdou, 2013*a*,*b*, 2017*a*,*b*,*c*, 2018; Abdou *et al.*, 2012*a*,*b*,*c*, 2013, 2015, 2015*a*,*b*, 2016; Abdou *et al.*, 2015*a*,*b*; Abdou, El-Saeed, Abozeid *et al.*, 2015;

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1H···O2^{i}	0.86 (3)	1.96 (4)	2.805 (3)	169 (3)

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

Metwally *et al.*, 2012*a*,*b*, 2013), we report herein the crystal structure of methyl 3-(2-hydroxyphenyl)propionate.

The molecular structure of the title compound is depicted in Fig. 1. The phenyl ring is planar with the hydroxyl group being coplanar with a C2—C1—O1—H1H torsion angle of −8 (2)°. The bond distances and angles within the phenolic ring, the propionate group and the co-planarity of OH group with the phenyl ring are consistent with related structures such as methyl 3-(3,5-di-tertbutyl-4-hydroxyphenyl)propionate (Li *et al.*, 2014), 2-(4-acetylanilino)-2-oxoethyl 3-(4-hydroxyphenyl)-propionate (Ashraf *et al.*, 2016) and methyl 3-[3-*tert*-butyl-5-(6-chloro-1-oxybenzotriazol-2-yl)-4-hydroxyphenyl]propionate (Wen *et al.*, 2006).

The crystal structure exhibits significant hydrogen-bonding interactions (Table 1), in which the O1—H1 groups acts as the donor while the carbonyl group of an adjacent molecule ($-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$) being the acceptor. These hydrogen bonds shown as dashed lines in Fig. 2) connect the molecules into chains running parallel to the *b* axis (Fig. 3). π–π stacking and C—H···π interactions are not present in the crystal structure.

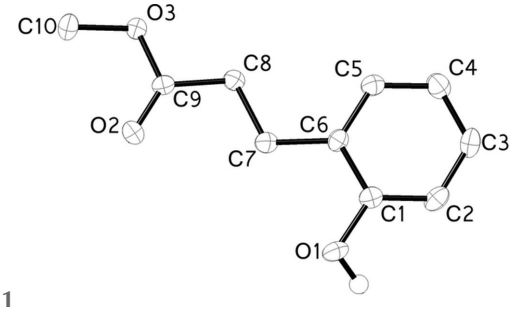


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

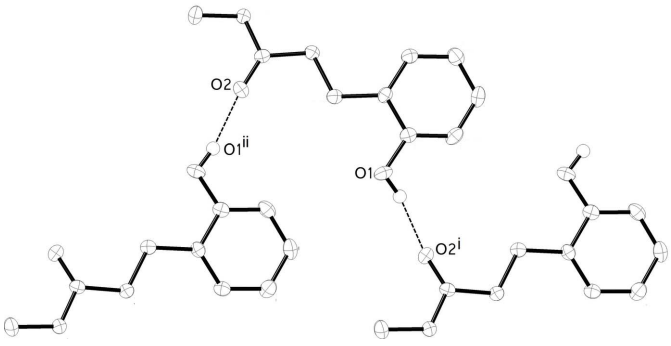


Figure 2
Hydrogen-bonding interactions (dashed lines) between adjacent molecules. Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_{12}O_3$
M_r	180.20
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	180
a, b, c (Å)	5.4774 (6), 11.1557 (12), 14.5610 (17)
V (Å^3)	889.74 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.35 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker D8 Venture diffractometer with PHOTON 100 CMOS detecter
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.614, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9443, 1756, 1390
R_{int}	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.091, 1.04
No. of reflections	1756
No. of parameters	122
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.15
Absolute structure	Flack x determined using 467 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.5 (8)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXS97* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2018* (Sheldrick, 2015).

Synthesis and crystallization

A mixture of dihydrocoumarin (1 ml, 7.89 mmol), a catalytic amount of conc. H_2SO_4, and 30 ml of dry MeOH were heated under reflux for 5 h. The methanol was removed *in vacuo* and the residue was neutralized with saturated $NaHCO_3$ solution then diluted with water and extracted with Et_2O. The combined organic extracts were dried over $MgSO_4$, filtered and concentrated. The crude compound was crystallized by slow evaporation of a diethyl ether–hexane mixture (2:1 *v*/*v*)

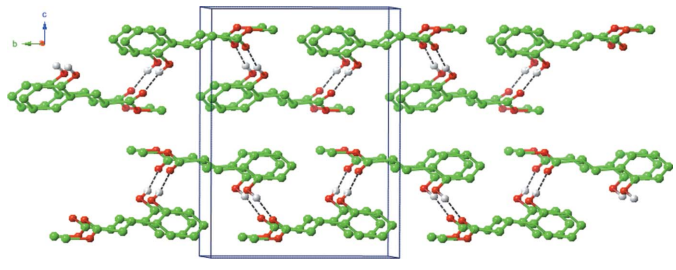


Figure 3
Crystal packing of the title compound viewed along the *a* axis, showing the chains parallel to the *a* axis formed *via* hydrogen bonding (dashed lines).

to give colourless single crystals (1.22 g, 86%). M.p. 41–42°C; IR (KBr, cm^{-1}) 3420, 3055, 1735, 1447. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.76 (*t*, *J* = 6.6 Hz, 3H), 2.95 (*t*, *J* = 6.6 Hz, 2H), 3.72 (*s*, 3H), 6.89 (*d*, *J* = 7.4 Hz, 2H), 7.12–7.16 (*m*, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 24.86, 34.87, 52.24, 116.82, 120.81, 127.07, 128.23, 130.52, 154.26, 175.96. HRMS (ESI/QTOF) *m*/*z*: $[M]^+$ calculated for $C_{10}H_{12}O_3$ 180.0786, found 180.0774.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

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Methyl 3-(4-hydroxyphenyl)propionate

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Methyl 3-(4-hydroxyphenyl)propionate

Crystal data

$C_{10}H_{12}O_3$
M_r = 180.20
Orthorhombic, $P2_12_12_1$
a = 5.4774 (6) Å
b = 11.1557 (12) Å
c = 14.5610 (17) Å
V = 889.74 (17) Å^3
Z = 4
$F(000)$ = 384
D_x = 1.345 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2736 reflections
θ = 3.3–27.6°
μ = 0.10 mm^{-1}
T = 180 K
Block, colourless
0.35 × 0.15 × 0.10 mm

Data collection

Bruker D8 Venture diffractometer with PHOTON 100 CMOS detecter
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.614, T_{max} = 0.746
9443 measured reflections
1756 independent reflections
1390 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 26.0°, θ_{min} = 3.3°
h = −6→6
k = −13→13
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.091
S = 1.04
1756 reflections
122 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.1279P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack x determined using 467 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.5 (8)

Special details

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

Refinement. All hydrogen atoms on carbon atoms were calculated with C–H = 0.95, 0.98 and 0.99 Å for CH (aromatic), CH_2 and CH_3, respectively, and refined as riding atoms with $U_{iso}(H) = 1.2\ U_{eq}(C)$ for CH (aromatic) and CH_2, and 1.5 $U_{eq}(C)$ for CH_3. The H atoms of the –OH group was located in a differenceFourier map and refined without any constraint.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5468 (3)	0.18977 (17)	0.77139 (13)	0.0302 (5)
H1H	0.642 (6)	0.235 (3)	0.740 (2)	0.051 (11)*
O2	0.1249 (3)	−0.19195 (17)	0.84546 (13)	0.0304 (5)
O3	−0.2348 (3)	−0.18421 (16)	0.91771 (11)	0.0267 (5)
C1	0.3762 (5)	0.2573 (2)	0.81696 (17)	0.0220 (6)
C2	0.3865 (5)	0.3815 (2)	0.8200 (2)	0.0270 (7)
H2A	0.515418	0.422762	0.789969	0.032*
C3	0.2091 (5)	0.4451 (2)	0.86675 (19)	0.0293 (7)
H3A	0.215294	0.530216	0.868476	0.035*
C4	0.0235 (6)	0.3849 (2)	0.9108 (2)	0.0293 (7)
H4A	−0.097370	0.428212	0.943778	0.035*
C5	0.0136 (5)	0.2607 (2)	0.90690 (18)	0.0248 (6)
H5A	−0.115233	0.219904	0.937426	0.030*
C6	0.1866 (4)	0.1949 (2)	0.85970 (16)	0.0203 (6)
C7	0.1802 (5)	0.0596 (2)	0.85041 (19)	0.0251 (6)
H7A	0.191282	0.038987	0.784403	0.030*
H7B	0.326584	0.026163	0.881019	0.030*
C8	−0.0424 (5)	−0.0006 (2)	0.88985 (19)	0.0226 (6)
H8A	−0.055581	0.020109	0.955777	0.027*
H8B	−0.189442	0.030922	0.858512	0.027*
C9	−0.0375 (5)	−0.1341 (2)	0.88018 (19)	0.0209 (6)
C10	−0.2421 (5)	−0.3137 (2)	0.91727 (19)	0.0304 (7)
H10A	−0.393610	−0.341096	0.946253	0.046*
H10B	−0.235700	−0.342708	0.853791	0.046*
H10C	−0.101883	−0.345081	0.951474	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0222 (10)	0.0322 (11)	0.0363 (12)	−0.0049 (10)	0.0094 (9)	0.0037 (10)
O2	0.0278 (11)	0.0272 (10)	0.0362 (11)	0.0043 (9)	0.0102 (8)	−0.0033 (10)
O3	0.0245 (10)	0.0204 (9)	0.0353 (11)	−0.0020 (9)	0.0084 (8)	−0.0006 (9)
C1	0.0193 (16)	0.0266 (15)	0.0201 (14)	−0.0011 (12)	−0.0020 (12)	0.0008 (12)
C2	0.0226 (17)	0.0289 (16)	0.0296 (18)	−0.0085 (12)	−0.0028 (14)	0.0050 (12)
C3	0.0329 (16)	0.0195 (14)	0.0355 (17)	−0.0050 (13)	−0.0071 (14)	0.0006 (13)
C4	0.0290 (18)	0.0259 (16)	0.0329 (18)	0.0021 (13)	−0.0005 (15)	−0.0045 (12)
C5	0.0203 (16)	0.0265 (15)	0.0276 (16)	−0.0018 (12)	0.0029 (13)	0.0009 (12)
C6	0.0190 (13)	0.0213 (13)	0.0206 (14)	−0.0018 (12)	−0.0030 (11)	0.0018 (12)
C7	0.0226 (14)	0.0248 (15)	0.0278 (15)	0.0000 (12)	0.0048 (13)	0.0015 (13)
C8	0.0204 (14)	0.0223 (13)	0.0251 (14)	0.0015 (11)	0.0034 (12)	0.0013 (12)

C9	0.0200 (14)	0.0239 (14)	0.0188 (14)	0.0001 (12)	0.0016 (12)	0.0019 (11)
C10	0.0365 (16)	0.0195 (14)	0.0353 (16)	−0.0042 (14)	0.0031 (13)	0.0001 (13)

Geometric parameters (Å, º)

O1—C1	1.372 (3)	C5—C6	1.381 (4)
O1—H1H	0.86 (3)	C5—H5A	0.9500
O2—C9	1.210 (3)	C6—C7	1.516 (4)
O3—C9	1.334 (3)	C7—C8	1.506 (3)
O3—C10	1.445 (3)	C7—H7A	0.9900
C1—C2	1.387 (3)	C7—H7B	0.9900
C1—C6	1.397 (4)	C8—C9	1.496 (3)
C2—C3	1.382 (4)	C8—H8A	0.9900
C2—H2A	0.9500	C8—H8B	0.9900
C3—C4	1.377 (4)	C10—H10A	0.9800
C3—H3A	0.9500	C10—H10B	0.9800
C4—C5	1.388 (4)	C10—H10C	0.9800
C4—H4A	0.9500		
C1—O1—H1H	111 (2)	C8—C7—H7A	108.4
C9—O3—C10	116.1 (2)	C6—C7—H7A	108.4
O1—C1—C2	122.4 (3)	C8—C7—H7B	108.4
O1—C1—C6	116.6 (2)	C6—C7—H7B	108.4
C2—C1—C6	120.9 (3)	H7A—C7—H7B	107.5
C3—C2—C1	120.0 (3)	C9—C8—C7	113.2 (2)
C3—C2—H2A	120.0	C9—C8—H8A	108.9
C1—C2—H2A	120.0	C7—C8—H8A	108.9
C4—C3—C2	119.8 (3)	C9—C8—H8B	108.9
C4—C3—H3A	120.1	C7—C8—H8B	108.9
C2—C3—H3A	120.1	H8A—C8—H8B	107.8
C3—C4—C5	119.8 (3)	O2—C9—O3	122.9 (2)
C3—C4—H4A	120.1	O2—C9—C8	125.7 (2)
C5—C4—H4A	120.1	O3—C9—C8	111.4 (2)
C6—C5—C4	121.6 (3)	O3—C10—H10A	109.5
C6—C5—H5A	119.2	O3—C10—H10B	109.5
C4—C5—H5A	119.2	H10A—C10—H10B	109.5
C5—C6—C1	117.8 (2)	O3—C10—H10C	109.5
C5—C6—C7	123.9 (2)	H10A—C10—H10C	109.5
C1—C6—C7	118.3 (2)	H10B—C10—H10C	109.5
C8—C7—C6	115.4 (2)		
O1—C1—C2—C3	179.8 (2)	O1—C1—C6—C7	−1.6 (3)
C6—C1—C2—C3	0.8 (4)	C2—C1—C6—C7	177.5 (2)
C1—C2—C3—C4	0.5 (4)	C5—C6—C7—C8	5.0 (4)
C2—C3—C4—C5	−0.9 (4)	C1—C6—C7—C8	−174.0 (2)
C3—C4—C5—C6	0.1 (5)	C6—C7—C8—C9	−179.1 (2)
C4—C5—C6—C1	1.2 (4)	C10—O3—C9—O2	1.8 (4)
C4—C5—C6—C7	−177.9 (3)	C10—O3—C9—C8	−176.4 (2)

O1—C1—C6—C5	179.3 (2)	C7—C8—C9—O2	0.5 (4)
C2—C1—C6—C5	−1.6 (4)	C7—C8—C9—O3	178.6 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*H*···O2^{i}	0.86 (3)	1.96 (4)	2.805 (3)	169 (3)

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+3/2.