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3,4-Dimethoxyphenylacetic acid

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Key indicators

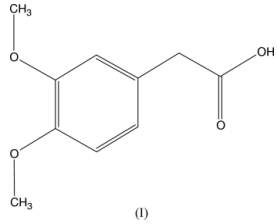
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.109
Data-to-parameter ratio = 12.5

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

The title compound, $C_{10}H_{12}O_4$, also known as homovaretic acid, forms hydrogen bonds, which generate chains rather than dimers in the crystal structure.

Comment

The title compound, (I), can be used as the starting material for the synthesis of a large number of 1,2,3,4-tetrahydroisoquinoline compounds (Nagarajan *et al.*, 1985). The molecules (Fig. 1) form O—H···O hydrogen bonds, resulting in an infinite chain along the crystallographic *b* axis (Figs. 2 and 3). It is noteworthy that 3-methoxyphenylacetic acid crystallizes in the same space group, but forms O—H···O hydrogen-bonded dimers (Choudhury & Guru Row, 2002). The torsion angles C4—C3—C2—C1 [−100.1 (1)°], C3—C2—C1—01 [86.2 (2)°] and C3—C2—C1—O2 [−90.8 (2)°] differ from those in 3-methoxyphenylacetic acid [88.1 (2), −0.2 (2) and 179.6 (1)°, respectively]. The two methoxy groups point away from each other [torsion angles C9—O3—C5— C6 = 175.6 (1)°, C10—O4—C6—C5 = 170.4 (1)° and O3—C5—C6—O4 = 1.3 (2)°]. The packing also involves two C—H···O hydrogen bonds (Table 1).



(I)

Experimental

The 98% pure compound was purchased from Sigma Aldrich. Single crystals were grown from a mixture of ethyl acetate and hexane at 283 K by slow evaporation.

Crystal data

$C_{10}H_{12}O_4$
M_r = 196.20
Monoclinic, $P2_1/c$
a = 14.258 (4) Å
b = 7.185 (2) Å
c = 9.773 (3) Å
β = 94.157 (5)°
V = 998.5 (5) Å^3
Z = 4
D_x = 1.305 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 541 reflections
θ = 6.2–21.1°
μ = 0.10 mm^{-1}
T = 293 (2) K
Prism, colourless
0.60 × 0.55 × 0.55 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.942, T_{max} = 0.947
7814 measured reflections
2193 independent reflections
1842 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 27.7°
$h = -18 \rightarrow 17$
$k = -9 \rightarrow 9$
$l = -12 \rightarrow 12$

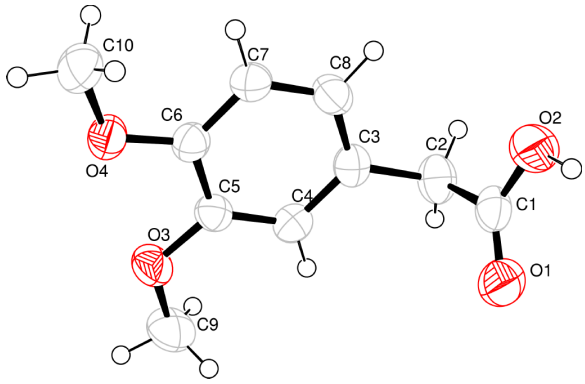


Figure 1
The molecular structure of the title compound, shown with 50% probability displacement ellipsoids.

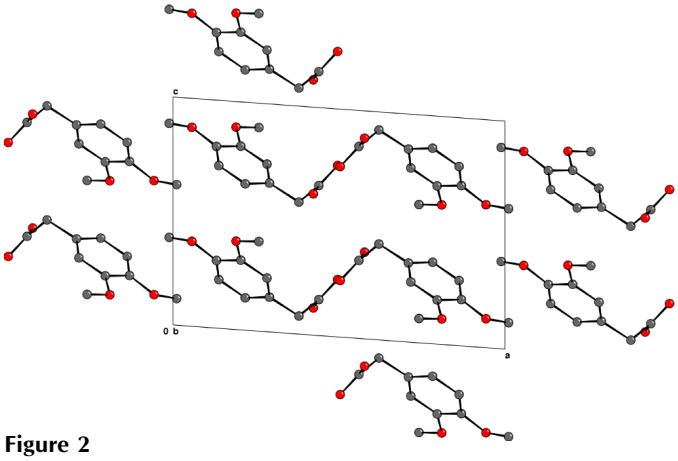


Figure 2
Packing diagram of the title compound, viewed down the *b* axis.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.196P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.041$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.109$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.19$ e Å^{-3}
2193 reflections	
175 parameters	
All H-atom parameters refined	

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H20···O1^{i}	0.94 (3)	1.73 (3)	2.651 (2)	163 (3)
C4—H4···O1^{ii}	0.940 (15)	2.583 (16)	3.473 (2)	158.2 (12)
C8—H8···O3^{iii}	0.977 (15)	2.592 (15)	3.537 (2)	162.7 (13)

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

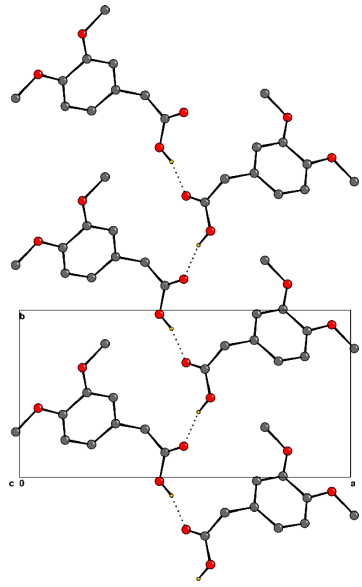


Figure 3
The hydrogen-bonded chains in (I), viewed down the *c* axis.

H atoms were located in a difference map and were refined isotropically. C—H distances are in the range 0.94 (2)–1.01 (2) Å and O—H is 0.95 (3) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 1998).

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