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2-(1,3-Benzodioxol-5-ylmethyl)acrylic acid

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In the title compound, $C_{11}H_{10}O_4$, the crystal packing is consolidated by O—H···O and C—H···O interactions.

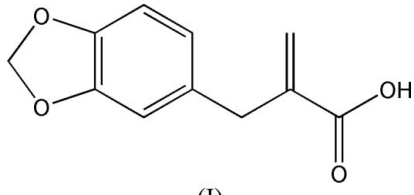
Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.151
Data-to-parameter ratio = 16.0

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

Comment

Fasidotril (Crosset & Danvy, 2003) is a potent dual ACE/NEP (angiotension-conversion enzyme/neutral endopeptidase) inhibitor for the prevention and treatment of hypertension and heart failure. The structure of the title compound, (I), an intermediate in the synthesis of fasidotril, is reported here.



(I)

As shown in Fig. 1, atoms C1/C2/C3/C4/O1/O2 are almost coplanar, with an r.m.s. deviation from the mean plane of 0.021 (2) Å. This plane is nearly orthogonal to the C5–C10 benzene ring plane, forming a dihedral angle of 84.34 (5)°.

In the crystal structure of (I), molecules are linked into inversion-related dimers by O2—H2···O1^{i} and O2^{i}—H2^{i}···O1 hydrogen bonds [symmetry code: (i) $-x, 1-y, -z$]. Two weak C—H···O interactions also occur (Table 1 and Fig. 2).

Experimental

The title compound was prepared following the procedure of Ebetino & Jorcai (2002). Colorless blocks of (I) were obtained by recrystallization from chloroform (m.p. 394 K).

Crystal data

$C_{11}H_{10}O_4$
M_r = 206.19
Triclinic, $P\overline{1}$
a = 4.9483 (8) Å
b = 9.0841 (12) Å
c = 11.7256 (16) Å
α = 111.881 (8)°
β = 91.747 (7)°
γ = 95.604 (8)°
V = 485.49 (12) Å^3
Z = 2
D_x = 1.410 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 113 (2) K
Block, colorless
0.24 × 0.22 × 0.12 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.975, T_{max} = 0.987
4479 measured reflections
2238 independent reflections
1270 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 27.9°
Standard reflections: ?

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.151$
$S = 0.94$
2238 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0796P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.36$ 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···O1^{i}	0.98 (2)	1.67 (3)	2.647 (2)	174 (2)
C3—H3B···O4^{ii}	0.95	2.59	3.217 (3)	124
C9—H9···O1^{iii}	0.95	2.56	3.239 (2)	128

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x, -y, -z$.

The O-bound H atom was located in a difference map. Its position was freely refined, with U_{iso}(H) = 1.5U_{eq}(O). The C-bound H atoms were positioned geometrically (C—H = 0.95–0.99 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure*; software used to prepare material for publication: *CrystalStructure*.

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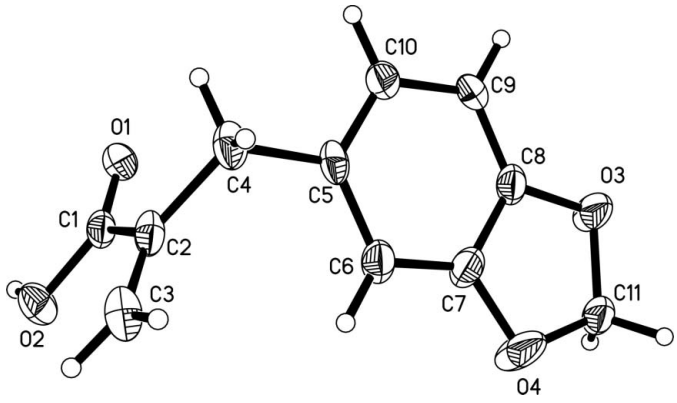

Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

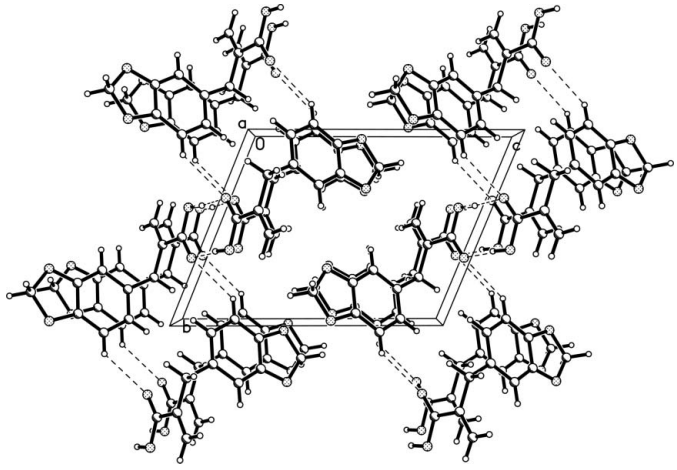

Figure 2
The packing of (I,) with hydrogen bonds shown as dashed lines.