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2-Hydroxycyclohexyl 1*H*-pyrrole-2-carboxylate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.112
Data-to-parameter ratio = 13.7

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

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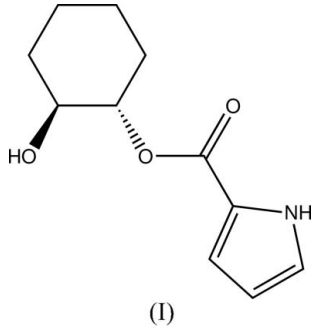
The molecule of the title compound, $C_{11}H_{15}NO_3$, bearing one pyrrolecarboxylate group and one hydroxyl group in an *anti* conformation, forms one-dimensional infinite pillars through intermolecular N—H···O and O—H···O hydrogen bonds between the pyrrolic NH, hydroxyl and carbonyl groups.

Comment

Hydrogen-bond-mediated self-assembly represents an area of considerable current interest (Burrows, 2004). It has recently been found that pyrrole-based entities are also capable of undergoing self-assembly through hydrogen bonds, especially in the solid state (Sessler *et al.*, 2003; Wang *et al.*, 2006; Yin *et al.*, 2006). Here we report the self-assembly of the title compound, (I), *via* conventional N—H···O and O—H···O hydrogen bonds. Treatment of *trans*-cyclohexane-1,2,-diol with 2-trichloroacetylpyrrole and triethylamine in refluxed acetonitrile solution gave the title compound directly. The molecular structure of (I) is shown in Fig. 1.



(I)

In the solid state, the cyclohexyl group adopts a chair conformation. The torsion angle between the pyrrole-2-carboxylate group and hydroxyl group, O3—C1—C6—O1, is

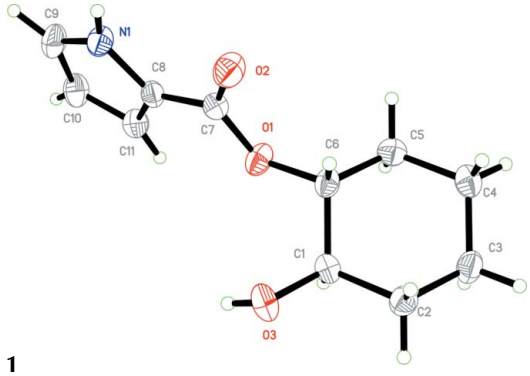


Figure 1
The molecular structure and numbering scheme of (I), with 30% probability ellipsoids.

62.34 (16)°. The pyrrole-2-carboxylate group is in a *syn* conformation, with the carbonyl group *syn* to its adjacent pyrrole NH group, while the pyrrole-2-carboxylate group is *anti* to its adjacent hydroxyl group.

In the crystal structure, two pyrrolic subunits are held together by a pair of N—H···O hydrogen bonds (Table 1) between the pyrrole and hydroxyl groups (Fig. 2). The dimers are further linked by a pair of O—H···O hydrogen bonds between the hydroxyl group and a carboxyl group from the second dimer, as shown in Fig. 3. Consequently, the molecules of (I) form one-dimensional infinite pillars.

Experimental

trans-Cyclohexane-1,2,-diol (116 mg, 1 mmol), 2-trichloroacetylpyrrole (211 mg, 1 mmol) and triethylamine (0.5 ml) were added to acetonitrile (20 ml), and the mixture was refluxed for 20 h. The solution was then evaporated under reduced pressure and the residue was purified by column chromatography on silica gel with ethyl acetate–petroleum ether (1:2 *v*/*v*), affording the title compound (white powder, 150 mg, 72%). Analysis: calculated for $C_{11}H_{15}NO_3$: C 63.14; H 7.23; N 6.69; found: C 63.25; H 7.33; N 6.58.

Crystal data

$C_{11}H_{15}NO_3$
M_r = 209.24
Triclinic, $P\overline{1}$
a = 5.266 (5) Å
b = 9.350 (8) Å
c = 11.932 (10) Å
α = 67.439 (11)°
β = 84.836 (12)°
γ = 85.742 (12)°
V = 539.8 (8) Å^3
Z = 2
D_x = 1.287 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colorless
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.757, T_{max} = 1.000
2938 measured reflections
1882 independent reflections
1382 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.03
1882 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0618P)^2 + 0.0534P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2^{i}	0.82	2.06	2.831 (2)	156
N1—H1···O3^{ii}	0.86	2.06	2.878 (3)	158

Symmetry codes: (i) $x+1, y, z$; (ii) $-x, -y+1, -z+2$.

All H atoms were located in a difference Fourier map, then refined as riding in their as-found relative positions (C—H =0.93, 0.97 or 0.98 Å, N—H = 0.82 Å and O—H =0.86 Å); U_{iso}(H) = 1.2U_{eq}(C).

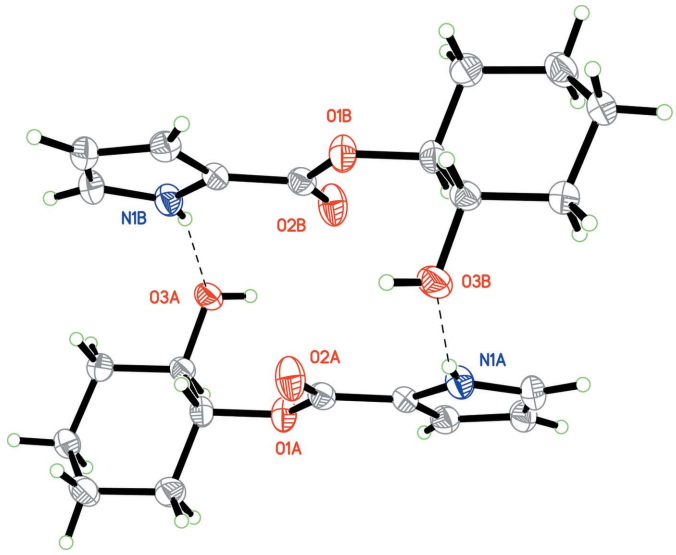


Figure 2
The dimer of molecules of (I) connected by N—H···O(−*x*, −*y* + 1, −*z* + 2) hydrogen bonds (dashed lines).

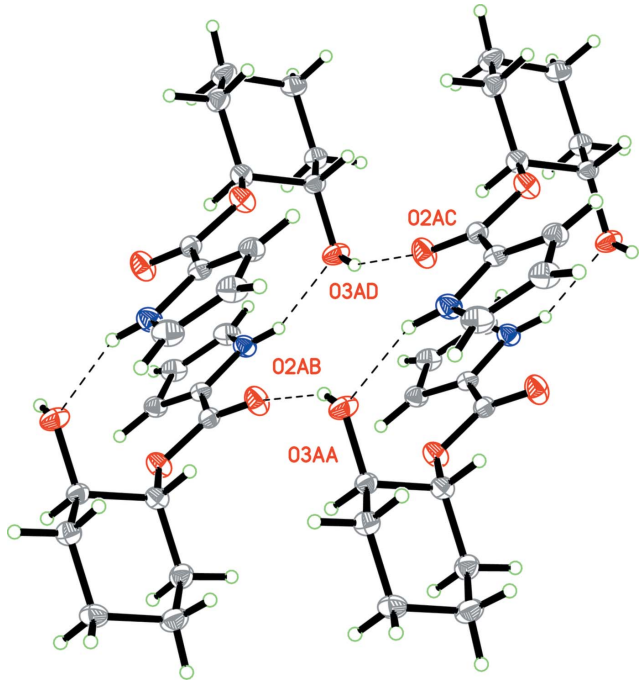


Figure 3
Dimers are held together *via* a pair of O—H···O(*x* + 1, *y*, *z*) hydrogen bonds (dashed lines).

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

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