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1,4-Dihydroxy-4-phenylbutan-2-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.125
Data-to-parameter ratio = 7.7

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

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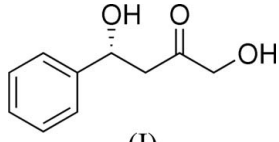
In the title compound, $C_{10}H_{12}O_3$, the butyl chain shows an extended planar conformation, and makes a dihedral angle of 73.98 (16)° with the benzene plane. The crystal packing is stabilized by O—H···O hydrogen bonding.

Comment

The title compound, (I), is an important intermediate for the construction of optically active 1,2,4-triols and substituted tetrahydrofuran (Chen *et al.*, 1987; Zheng *et al.*, 2005). Its crystal structure is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles in (I) are normal. The butyl chain shows an extended planar conformation, and makes a dihedral angle of 73.98 (16)° with the benzene plane. The crystal packing is stabilized by O—H···O hydrogen bonding (Table 1).

Experimental

Hydroxyacetone (0.5 ml) was added to a water/tetrahydrofuran solution (2 ml, 1:1) of benzaldehyde (53 mg, 0.5 mmol) and L-*N*-phenylpyrrolidine-2-carboxamide (19 mg, 20 mol%). The resulting mixture was stirred at 273 K for 4 d. The reaction mixture was treated with a saturated solution of ammonium chloride. The aqueous layer was extracted with ethyl acetate and dried over anhydrous $MgSO_4$. After filtration and removal of the solvent under reduced pressure, the residue was purified through column chromatography on silica gel to give (I). Colourless single crystals of (I) were obtained by recrystallization from an ethanol solution.

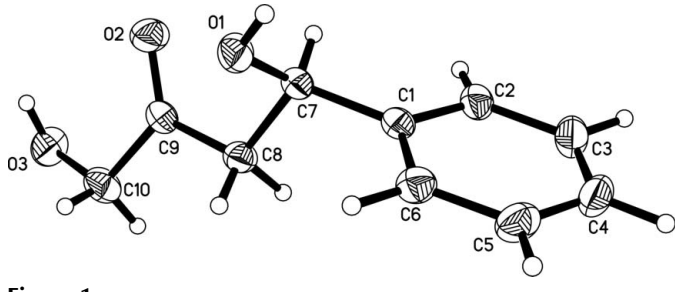


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Crystal data

$C_{10}H_{12}O_3$
M_r = 180.20
Monoclinic, $P2_1$
a = 7.9573 (13) Å
b = 5.4679 (15) Å
c = 11.043 (3) Å
β = 109.173 (16)°
V = 453.83 (19) Å^3
Z = 2
D_x = 1.319 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colourless
0.25 × 0.18 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1714 measured reflections
941 independent reflections
709 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 25.5°
3 standard reflections
every 250 reflections
intensity decay: 1.7%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.00
941 reflections
122 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0873P)^2 + 0.0008P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O3^{i}	0.82	1.94	2.759 (4)	175
O3—H3O···O1^{ii}	0.82	2.02	2.790 (4)	157

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

H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 Å (methylene) and O—H = 0.82 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C,O). In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *DIFRAC* (Gabe *et al.*, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia,1997); software used to prepare material for publication: *SHELXL97*.

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