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1,3-Benzodioxol-5-ylmethanol

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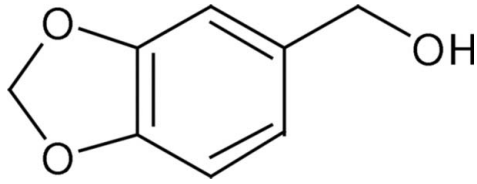
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.087; data-to-parameter ratio = 12.8.

The title compound, $C_8H_8O_3$, is an acid-protecting group used in the synthesis of peptides and as an accelerator in polymerization reactions. Its oxidation product, piperonal (heliotropine), is used in the flavouring and perfume industries. All the non-H atoms, except the O atom of the hydroxyl group, are coplanar (r.m.s. deviation 0.028 Å). The crystal packing is stabilized by an O—H···O hydrogen bond.

Related literature

For related structures, see: Viladomat *et al.* (1998); Nagaraj *et al.* (2005); Sonar *et al.* (2006); Harrison *et al.* (2006).

For related literature, see: Allen (2002); Bruno *et al.* (2004); Ortiz *et al.* (2005); Stewart (1971).



Experimental

Crystal data

$C_8H_8O_3$
M_r = 152.14
Monoclinic, $P2_1/c$
a = 13.544 (2) Å
b = 4.6718 (4) Å
c = 12.6416 (19) Å
β = 115.437 (11)°
V = 722.35 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 173 (2) K
0.42 × 0.38 × 0.37 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: none
3862 measured reflections
1342 independent reflections
1221 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.088
S = 1.04
1342 reflections
105 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1^{i}	0.91 (2)	1.82 (2)	2.7256 (9)	173.2 (18)

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2362).

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supplementary materials

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1,3-Benzodioxol-5-ylmethanol

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Comment

The title compound, (I), is an acid-protecting group used in the synthesis of peptides (Stewart, 1971) and as an accelerator in polymerization reactions (Ortiz *et al.*, 2005). Its oxidation product, piperonal (heliotropine) is used in the flavouring and perfume industry.

A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal [Cambridge Structural Database, Version 5.28, November 2006,

updated January 2007 (Allen, 2002); Mogul, Version 1.1 (Bruno *et al.*, 2004)]. All the non-H atoms of the molecule, except the hydroxyl O atom, lie in a common plane (r.m.s. deviation 0.028 Å). The hydroxyl O atom deviates by

0.529 (1) Å from this plane.

The crystal packing is stabilized by an O—H···O hydrogen bond (Table 1 and Fig. 2).

Experimental

The title compound was obtained as a gift sample from Arvee Chem Pharma, Mysore, India. X-ray quality crystals of (I) were obtained from a solution in acetonitrile after slow evaporation (m.p. 329 K).

Refinement

H atoms were found in a difference map, but those bonded to C atoms were relocated in idealised locations and refined using a riding model, with $C_{aromatic}$—H = 0.95 Å or $C_{methylene}$—H = 0.99 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. The hydroxyl H atom was refined freely.

Figures

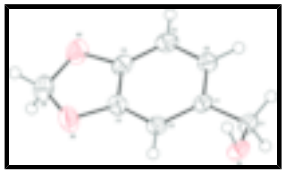

Fig. 1. A perspective view of (I), with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for H atoms).

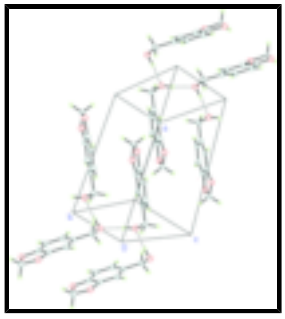

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

1,3-Benzodioxol-5-ylmethanol

Crystal data

$C_8H_8O_3$	F_{000} = 320
M_r = 152.14	D_x = 1.399 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3407 reflections
a = 13.544 (2) Å	θ = 3.7–25.6º
b = 4.6718 (4) Å	μ = 0.11 mm^{-1}
c = 12.6416 (19) Å	T = 173 (2) K
β = 115.437 (11)º	Block, colourless
V = 722.35 (18) Å^3	0.42 × 0.38 × 0.37 mm
Z = 4	

Data collection

Stoe IPDSII two-circle diffractometer	1221 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.024
Monochromator: graphite	θ_{max} = 25.6º
T = 173(2) K	θ_{min} = 3.6º
ω scans	h = −16→14
Absorption correction: none	k = −5→5
3862 measured reflections	l = −15→15
1342 independent reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.1849P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.088	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.13 e Å^{-3}

1342 reflections

105 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.038 (5)

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. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.05317 (7)	0.13672 (19)	0.29543 (7)	0.0307 (3)
H1	0.0202 (16)	0.309 (5)	0.2709 (16)	0.064 (5)*
O2	0.40248 (8)	0.7637 (2)	0.50957 (8)	0.0466 (3)
O3	0.40887 (8)	0.9045 (2)	0.68892 (8)	0.0413 (3)
C1	0.16608 (9)	0.3348 (2)	0.49175 (9)	0.0237 (3)
C2	0.24400 (10)	0.4373 (3)	0.45489 (10)	0.0278 (3)
H2	0.2437	0.3780	0.3829	0.033*
C3	0.32085 (10)	0.6276 (3)	0.52810 (10)	0.0288 (3)
C4	0.32402 (9)	0.7128 (3)	0.63447 (10)	0.0289 (3)
C5	0.24944 (10)	0.6147 (3)	0.67288 (10)	0.0313 (3)
H5	0.2517	0.6729	0.7459	0.038*
C6	0.16949 (10)	0.4234 (3)	0.59852 (10)	0.0278 (3)
H6	0.1161	0.3524	0.6219	0.033*
C7	0.07960 (10)	0.1216 (2)	0.41779 (10)	0.0273 (3)
H7A	0.1056	−0.0740	0.4462	0.033*
H7B	0.0123	0.1557	0.4285	0.033*
C8	0.46503 (11)	0.9200 (3)	0.61560 (12)	0.0400 (3)
H8A	0.5390	0.8357	0.6564	0.048*
H8B	0.4729	1.1221	0.5970	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0408 (5)	0.0245 (5)	0.0225 (4)	0.0006 (4)	0.0095 (4)	−0.0013 (3)
O2	0.0419 (6)	0.0602 (7)	0.0433 (6)	−0.0214 (5)	0.0235 (5)	−0.0135 (5)
O3	0.0384 (5)	0.0441 (6)	0.0354 (5)	−0.0124 (4)	0.0104 (4)	−0.0105 (4)

C1	0.0271 (6)	0.0186 (5)	0.0231 (5)	0.0045 (4)	0.0085 (4)	0.0038 (4)
C2	0.0334 (6)	0.0276 (6)	0.0234 (6)	0.0013 (5)	0.0130 (5)	−0.0010 (5)
C3	0.0274 (6)	0.0298 (6)	0.0295 (6)	0.0004 (5)	0.0125 (5)	0.0023 (5)
C4	0.0292 (6)	0.0255 (6)	0.0250 (6)	0.0000 (5)	0.0049 (5)	−0.0016 (5)
C5	0.0402 (7)	0.0308 (7)	0.0221 (6)	0.0018 (5)	0.0128 (5)	−0.0019 (5)
C6	0.0328 (6)	0.0266 (6)	0.0259 (6)	0.0017 (5)	0.0145 (5)	0.0026 (4)
C7	0.0342 (6)	0.0214 (6)	0.0238 (6)	0.0001 (5)	0.0099 (5)	0.0029 (4)
C8	0.0344 (7)	0.0417 (8)	0.0383 (7)	−0.0099 (6)	0.0103 (6)	−0.0020 (6)

Geometric parameters (Å, °)

O1—C7	1.4319 (14)	C2—H2	0.9500
O1—H1	0.91 (2)	C3—C4	1.3854 (17)
O2—C3	1.3799 (15)	C4—C5	1.3740 (17)
O2—C8	1.4393 (16)	C5—C6	1.4072 (17)
O3—C4	1.3845 (15)	C5—H5	0.9500
O3—C8	1.4314 (18)	C6—H6	0.9500
C1—C6	1.3935 (16)	C7—H7A	0.9900
C1—C2	1.4078 (16)	C7—H7B	0.9900
C1—C7	1.5158 (16)	C8—H8A	0.9900
C2—C3	1.3794 (17)	C8—H8B	0.9900
C7—O1—H1	105.7 (12)	C6—C5—H5	121.7
C3—O2—C8	105.65 (10)	C1—C6—C5	122.11 (11)
C4—O3—C8	105.61 (9)	C1—C6—H6	118.9
C6—C1—C2	120.13 (11)	C5—C6—H6	118.9
C6—C1—C7	119.20 (10)	O1—C7—C1	113.72 (9)
C2—C1—C7	120.65 (10)	O1—C7—H7A	108.8
C3—C2—C1	117.00 (10)	C1—C7—H7A	108.8
C3—C2—H2	121.5	O1—C7—H7B	108.8
C1—C2—H2	121.5	C1—C7—H7B	108.8
C2—C3—O2	127.73 (11)	H7A—C7—H7B	107.7
C2—C3—C4	122.44 (11)	O3—C8—O2	108.28 (10)
O2—C3—C4	109.82 (11)	O3—C8—H8A	110.0
C5—C4—O3	128.27 (11)	O2—C8—H8A	110.0
C5—C4—C3	121.74 (11)	O3—C8—H8B	110.0
O3—C4—C3	109.98 (11)	O2—C8—H8B	110.0
C4—C5—C6	116.58 (11)	H8A—C8—H8B	108.4
C4—C5—H5	121.7		
C6—C1—C2—C3	−0.71 (17)	O2—C3—C4—O3	−0.76 (14)
C7—C1—C2—C3	−179.07 (10)	O3—C4—C5—C6	178.68 (11)
C1—C2—C3—O2	−177.66 (11)	C3—C4—C5—C6	−0.12 (18)
C1—C2—C3—C4	1.18 (18)	C2—C1—C6—C5	−0.15 (18)
C8—O2—C3—C2	−175.52 (13)	C7—C1—C6—C5	178.22 (10)
C8—O2—C3—C4	5.52 (14)	C4—C5—C6—C1	0.57 (18)
C8—O3—C4—C5	176.71 (13)	C6—C1—C7—O1	155.02 (10)
C8—O3—C4—C3	−4.37 (14)	C2—C1—C7—O1	−26.61 (15)
C2—C3—C4—C5	−0.78 (19)	C4—O3—C8—O2	7.72 (14)
O2—C3—C4—C5	178.24 (11)	C3—O2—C8—O3	−8.18 (14)
C2—C3—C4—O3	−179.79 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1^{i}	0.91 (2)	1.82 (2)	2.7256 (9)	173.2 (18)

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

Fig. 1

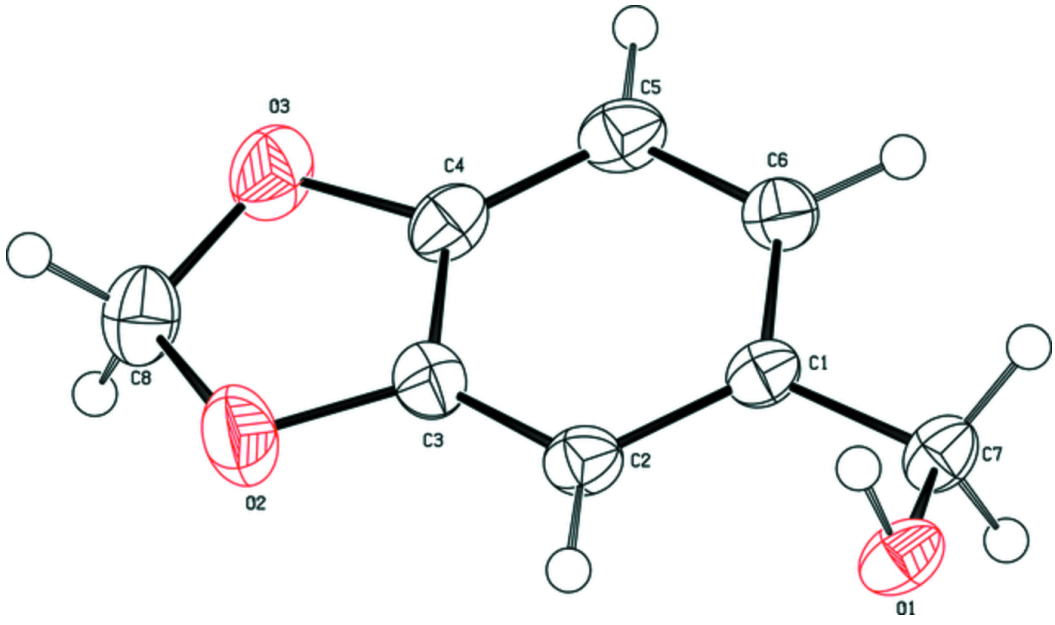

Fig. 2