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3-(2-Methoxyphenoxy)propane-1,2-diol

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Key indicators

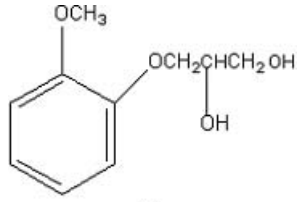
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.148
Data-to-parameter ratio = 17.7

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

The title compound, $C_{10}H_{14}O_4$, is used to cure coughs and clear up phlegm and it is also used as an intermediate in the synthesis of other medicinal products. The entire molecule, except for atoms C10 and O4, is essentially planar (to within 0.001 Å).

Comment

The title compound, (I), also known as guaiphenesin, is an ingredient usually found in cold preparations. In the year 1530, it was first extracted from guaiacum and used to treat rheumatism. Over 20 years ago, it was synthesized, named guaiphenesin, and pressed into tablets (Starlanyl, 2001). To the best of our knowledge [using Chemical Abstracts and the Cambridge Structural Database (Allen, 2002)], the single-crystal structure has not been reported previously.



(I)

The molecular structure of (I) is shown in Fig. 1. It can be seen that the entire molecule, except for atoms C10 and O4

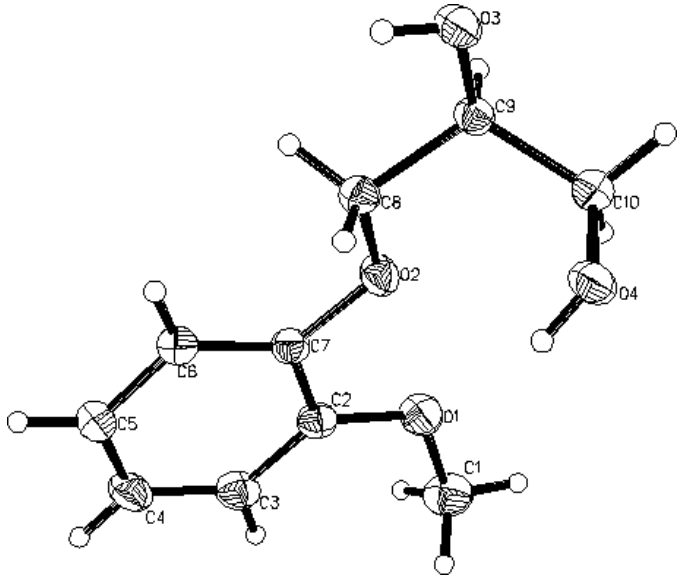


Figure 1
ORTEPII (Johnson, 1976) view of the title compound, (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

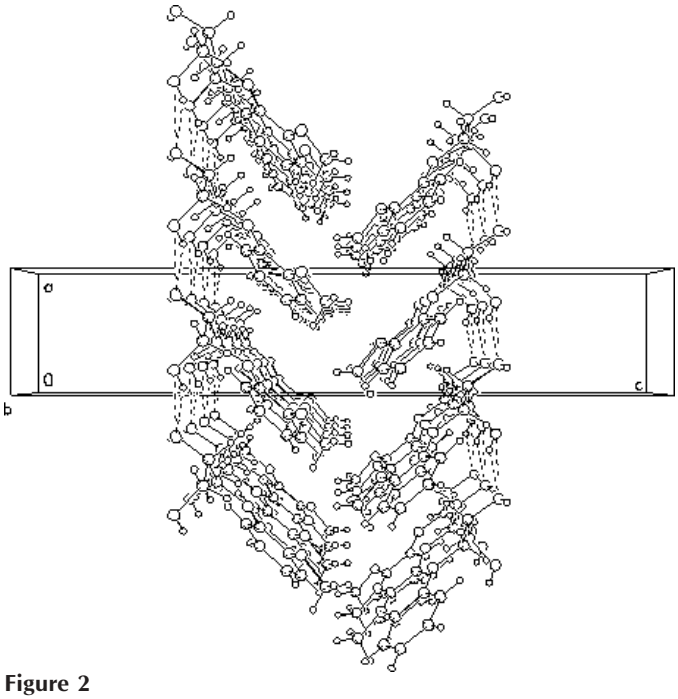


Figure 2
The molecular packing of compound (I), viewed along the *b* axis.

and the H atoms, is essentially planar (to within 0.001 Å). The crystal packing projected on to the *ac* face is shown in Fig. 2. There are two kinds of intermolecular hydrogen bonds between molecules (Table 1). The hydrogen bond O3—H3···O4 is approximately parallel to the *ac* face, while O4—H4···O3 is approximately perpendicular to the *ac* face.

Experimental

The title compound was provided by Tianjin Zhongxin Pharmaceutical Co. Ltd. A saturated solution of guaiphenesin in ethanol was prepared at 338–343 K and then a small quantity of seeds was added when the temperature fell to 308 K. After a long time, a large quantity of white crystals was obtained by recrystallization. The product was characterized by NMR, IR and elemental analyses, and its purity was 99%. The melting point determined by DSC (differential scanning calorimetry) is 355.4 K. Colorless block-shaped single crystals suitable for X-ray diffraction were obtained by adding a small quantity of seeds to a room-temperature solution of the above product and placing it in a refrigerator for 3 d.

Crystal data

$C_{10}H_{14}O_4$
M_r = 198.21
Orthorhombic, $P2_12_12_1$
a = 4.9836 (10) Å
b = 7.6562 (15) Å
c = 25.698 (5) Å
V = 980.5 (3) Å^3
Z = 4
D_x = 1.343 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9593 reflections
θ = 3.1–27.5°
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colorless
0.38 × 0.20 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.962, T_{max} = 0.991
9631 measured reflections
2248 independent reflections
1862 reflections with $I > 2\sigma(I)$
R_{int} = 0.092
θ_{max} = 27.5°
$h = -6 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -33 \rightarrow 32$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.148
S = 1.00
2248 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0903P)^2 + 0.0695P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···O4^{i}	0.82	1.96	2.744 (2)	161
O4—H4C···O3^{ii}	0.82	1.99	2.729 (2)	149

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

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous dispersion effects, Friedel equivalents were merged prior to the final refinements, and the absolute configuration was assigned to correspond with the known chiral centers of the precursor molecule, which remained unchanged during the synthesis of the title compound.

Data collection: *RAPID-AUTO* (Rigaku, 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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