Crystal structure of *erythro*-1-(4-benzyloxy-3-methoxyphenyl)-2-(4-hydroxy-3-methoxyphenyl)-1,3-propanediol, C₂₄H₂₆O₆

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Table 1. Parameters used for the X-ray data collection

Crystal:	colorless prism, size 0.24 x 0.40 x 0.57 mm
Wavelength:	Mo K α radiation (0.71069 Å)
μ :	0.92 cm ⁻¹
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	53°
$N(hkl)_{\text{unique}}$:	4286
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	376
Programs:	SHELXS-86, SHELXL-93

Source of material: The title compound was prepared starting from 1-(4-benzyloxy-3-methoxyphenyl)-1-ethanone and the tetrahydropyran-2-yl ether of vanillin using a procedure earlier applied for the synthesis of an isomeric compound (see ref. 1). Crystals were obtained from ethyl acetate (mp 396–397 K). The crystal structure determination demonstrates that the title compound has the *erythro*-configuration. The torsion angle C1–C7–C8–C11 is $-49.8(2)^\circ$. The structure is stabilized by intermolecular hydrogen bonds [O1...O4=2.751(2) Å, O1–H1A...O4=158°; O2...O1= 2.709(2) Å, O2–H2A...O1=174°; O4...O2=2.663(3) Å, O4–H4A...O2= 169°]. ¹H NMR spectrum (400 MHz, DMSO-*d*₆, TMS, 20 °C): δ 2.75 [1H, m; H(C8)], 3.61 and 3.63 (OCH₃), 3.47 (1H, m) and 3.67 (1H, m) [H(C9)], 4.44 (1H, t, $J=5.0$ Hz; OH), 4.87 [1H, d, $J=4.8$ Hz; H(C7)], $\sim$ 5.0 (1H; OH), 5.01(2H, s, Ph–CH₂–O), 6.4–7.5 (11 H, m; H–Ar) and 8.59 (ArOH). Crystal structures of two related compounds have previously been reported (see refs. 2 and 3).

C₂₄H₂₆O₆, triclinic, $P\bar{1}$ (No. 2), $a=6.6821(5)$ Å, $b=9.2393(7)$ Å, $c=18.679(2)$ Å, $\alpha=82.490(2)^\circ$, $\beta=86.992(2)^\circ$, $\gamma=67.363(2)^\circ$, $V=1055.2$ Å³, $Z=2$, $R(F)=0.037$, $R_w(F^2)=0.091$.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
H(1)	2i	0.063(3)	0.024(2)	−0.2249(9)	0.041(5)
H(2)	2i	−0.689(3)	0.280(2)	−0.197(1)	0.054(5)
H(3)	2i	−0.533(3)	0.232(2)	−0.312(1)	0.044(5)
H(4)	2i	−0.008(3)	−0.014(2)	−0.3495(8)	0.034(4)
H(5)	2i	0.127(3)	0.169(2)	−0.3489(8)	0.033(4)
H(6)	2i	0.177(3)	0.235(2)	−0.474(1)	0.048(5)
H(7)	2i	−0.040(3)	0.212(2)	−0.4957(9)	0.038(4)
H(8)	2i	0.167(4)	−0.147(3)	−0.113(1)	0.069(7)
H(9)	2i	0.250(5)	−0.005(3)	−0.127(2)	0.098(9)
H(10)	2i	0.212(3)	−0.077(2)	−0.042(1)	0.064(6)
H(11)	2i	0.101(3)	0.412(2)	−0.3282(9)	0.040(5)
H(12)	2i	−0.583(3)	0.676(2)	−0.435(1)	0.045(5)
H(13)	2i	−0.406(3)	0.404(2)	−0.436(1)	0.051(5)
H(14)	2i	0.112(4)	0.574(3)	−0.238(1)	0.081(7)
H(15)	2i	0.245(4)	0.591(3)	−0.311(1)	0.074(7)
H(16)	2i	0.164(3)	0.734(3)	−0.263(1)	0.067(6)
H(17)	2i	−0.722(4)	0.408(3)	−0.095(1)	0.079(7)
H(18)	2i	−0.791(4)	0.259(3)	−0.076(1)	0.085(8)
H(19)	2i	−0.687(4)	0.118(3)	0.055(1)	0.074(7)
H(20)	2i	−0.682(5)	0.152(4)	0.181(2)	0.12(1)
H(21)	2i	−0.713(5)	0.397(3)	0.210(2)	0.110(9)
H(22)	2i	−0.742(5)	0.599(4)	0.119(2)	0.11(1)
H(23)	2i	−0.745(4)	0.565(3)	−0.004(1)	0.079(7)
H(1A)	2i	−0.330(7)	0.016(5)	−0.391(2)	0.17(2)
H(2A)	2i	0.211(5)	−0.020(4)	−0.505(2)	0.12(1)
H(4A)	2i	−0.576(5)	0.916(4)	−0.413(2)	0.12(1)

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(1)	2i	-0.2800(2)	0.0992(1)	-0.40411(6)	0.0552(8)	0.0430(7)	0.0358(6)	-0.0216(6)	-0.0055(5)	-0.0093(5)
O(2)	2i	0.1997(2)	0.0104(1)	-0.46290(7)	0.0460(7)	0.0400(7)	0.0427(7)	-0.0005(5)	-0.0019(6)	-0.0186(6)
O(3)	2i	-0.0642(2)	0.7235(1)	-0.32055(7)	0.0525(8)	0.0297(6)	0.0736(9)	-0.0121(6)	-0.0229(7)	-0.0071(6)
O(4)	2i	-0.4515(2)	0.8664(1)	-0.37949(8)	0.0483(7)	0.0238(6)	0.0731(9)	-0.0032(5)	-0.0178(7)	-0.0070(6)
O(5)	2i	-0.0616(2)	0.0583(2)	-0.08873(6)	0.0492(7)	0.0634(8)	0.0310(6)	-0.0059(6)	-0.0050(5)	-0.0080(6)
O(6)	2i	-0.4705(2)	0.2059(2)	-0.07355(6)	0.0510(7)	0.0523(7)	0.0349(7)	-0.0045(6)	0.0085(5)	-0.0068(5)
C(1)	2i	-0.2234(3)	0.1260(2)	-0.28028(8)	0.0433(9)	0.0262(8)	0.0310(8)	-0.0111(7)	-0.0001(7)	-0.0031(6)
C(2)	2i	-0.0909(3)	0.0768(2)	-0.21927(9)	0.0366(9)	0.0336(8)	0.0339(8)	-0.0079(7)	-0.0008(7)	-0.0050(6)
C(3)	2i	-0.1775(3)	0.1038(2)	-0.15138(8)	0.046(1)	0.0328(8)	0.0314(8)	-0.0106(7)	-0.0030(7)	-0.0038(6)
C(4)	2i	-0.4022(3)	0.1829(2)	-0.14297(8)	0.046(1)	0.0336(8)	0.0313(8)	-0.0097(7)	0.0057(7)	-0.0052(6)
C(5)	2i	-0.5329(3)	0.2296(2)	-0.2029(1)	0.040(1)	0.046(1)	0.042(1)	-0.0062(8)	0.0021(8)	-0.0042(8)
C(6)	2i	-0.4430(3)	0.2007(2)	-0.27108(9)	0.043(1)	0.0416(9)	0.0360(9)	-0.0068(8)	-0.0059(8)	-0.0025(7)
C(7)	2i	-0.1216(3)	0.0935(2)	-0.35387(8)	0.0433(9)	0.0264(8)	0.0300(8)	-0.0084(7)	-0.0028(7)	-0.0060(6)
C(8)	2i	-0.0060(3)	0.2043(2)	-0.38346(8)	0.0370(9)	0.0259(8)	0.0304(8)	-0.0062(7)	-0.0032(7)	-0.0045(6)
C(9)	2i	0.0801(3)	0.1750(2)	-0.45984(9)	0.042(1)	0.0330(9)	0.0331(9)	-0.0073(7)	0.0003(7)	-0.0063(7)
C(10)	2i	0.1583(4)	-0.0498(3)	-0.0919(1)	0.052(1)	0.075(2)	0.040(1)	-0.005(1)	-0.009(1)	-0.005(1)
C(11)	2i	-0.1333(2)	0.3800(2)	-0.38195(8)	0.0378(8)	0.0259(7)	0.0275(8)	-0.0087(6)	0.0015(6)	-0.0034(6)
C(12)	2i	-0.0416(3)	0.4677(2)	-0.35011(8)	0.0350(9)	0.0286(8)	0.0358(8)	-0.0073(7)	-0.0039(7)	-0.0027(6)
C(13)	2i	-0.1447(3)	0.6292(2)	-0.34999(8)	0.0395(9)	0.0299(8)	0.0373(9)	-0.0136(7)	-0.0024(7)	-0.0057(6)
C(14)	2i	-0.3485(3)	0.7067(2)	-0.38176(9)	0.0389(9)	0.0237(7)	0.0395(9)	-0.0065(7)	-0.0018(7)	-0.0029(6)
C(15)	2i	-0.4403(3)	0.6217(2)	-0.4138(1)	0.0382(9)	0.0326(9)	0.048(1)	-0.0078(7)	-0.0105(8)	-0.0031(7)
C(16)	2i	-0.3346(3)	0.4595(2)	-0.41415(9)	0.0429(9)	0.0300(8)	0.045(1)	-0.0118(7)	-0.0088(8)	-0.0056(7)
C(17)	2i	0.1318(3)	0.6494(3)	-0.2808(1)	0.046(1)	0.045(1)	0.076(2)	-0.0140(9)	-0.016(1)	-0.013(1)
C(18)	2i	-0.6921(3)	0.3077(3)	-0.0621(1)	0.049(1)	0.059(1)	0.048(1)	-0.006(1)	0.0100(9)	-0.013(1)
C(19)	2i	-0.7095(3)	0.3367(2)	0.0154(1)	0.044(1)	0.047(1)	0.052(1)	-0.0142(8)	0.0151(8)	-0.0151(8)
C(20)	2i	-0.6960(4)	0.2169(3)	0.0696(1)	0.075(2)	0.053(1)	0.053(1)	-0.028(1)	0.017(1)	-0.017(1)
C(21)	2i	-0.6985(4)	0.2388(3)	0.1414(1)	0.089(2)	0.084(2)	0.051(1)	-0.039(2)	0.022(1)	-0.018(1)
C(22)	2i	-0.7158(4)	0.3816(4)	0.1590(2)	0.088(2)	0.115(2)	0.063(2)	-0.060(2)	0.034(1)	-0.046(2)
C(23)	2i	-0.7355(5)	0.5035(4)	0.1061(2)	0.095(2)	0.087(2)	0.106(2)	-0.056(2)	0.046(2)	-0.063(2)
C(24)	2i	-0.7310(4)	0.4813(3)	0.0340(1)	0.075(2)	0.054(1)	0.080(2)	-0.030(1)	0.029(1)	-0.019(1)

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