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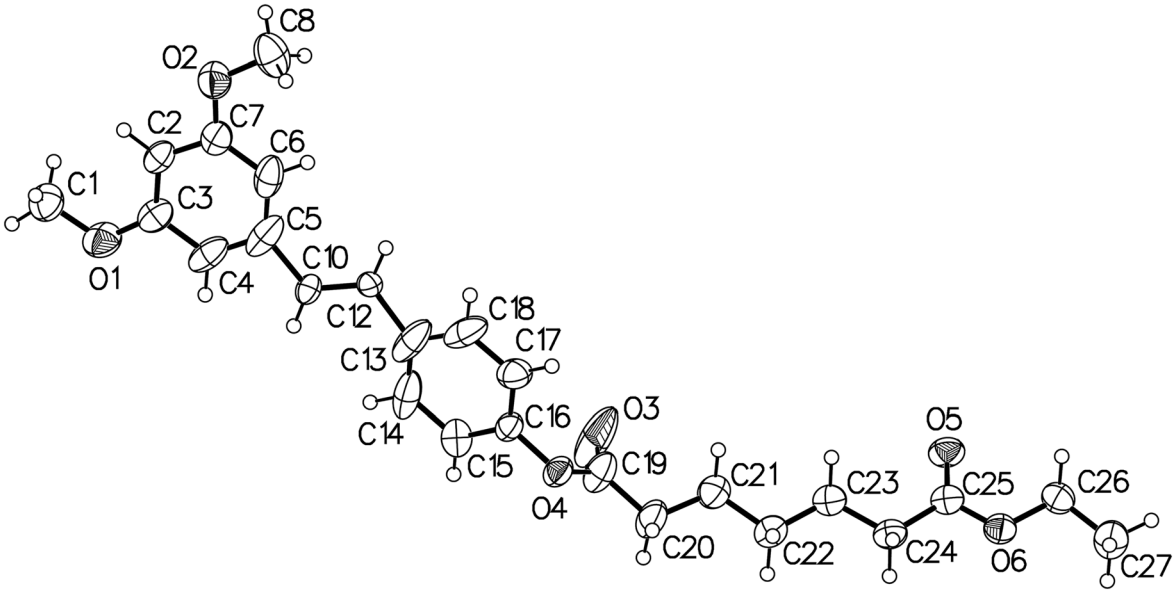
Crystal structure of (*E*)-1-(4-(3,5-dimethoxystyryl) phenyl)-7-ethylheptanedioate, $C_{25}H_{30}O_6$



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Abstract

$C_{25}H_{30}O_6$, orthorhombic, $Pna2_1$ (no. 33), a = 7.556(2) Å, b = 37.198(12) Å, c = 8.113(2) Å, V = 2280.2(11) Å^3, Z = 4, $R_{gt}(F)$ = 0.0610, $wR_{ref}(F^2)$ = 0.1634, T = 170 K.

CCDC no.: 2161245

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.11 × 0.08 × 0.05 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	26.4°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11,367, 4039, 0.081
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3087
$N(param)_{refined}$:	301
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

Source of material

The compound (*E*)-4-(3,5-dimethoxystyryl)phenol (2 mmol) was dissolved in dichloromethane (10 mL), and then 7-ethoxy-7-oxoheptanoic acid (2 mmol), 2-(7-azabenzotriazol-1-yl)-*N*,*N*,*N*′,*N*′-tetramethyluronium hexafluorophosphate (HATU, 2 mmol), and *N*,*N*-diisopropylethylamine (DIEA, 4 mmol) were added to the mixture successively with stirring. The reaction was maintained for 4 h at room temperature and monitored by thin-layer chromatography. The mixture was concentrated under reduced pressure after the reaction was completed. The crude product was separated and purified by silica gel column chromatography with petroleum ether and ethyl acetate (v/v = 10/1) as eluent. We obtained a white solid with a yield of 82.1%. Subsequently, the title compound

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	1.7461 (7)	0.72290 (14)	0.3544 (8)	0.0627 (13)
H1A	1.797222	0.714591	0.458672	0.094*
H1B	1.700900	0.747408	0.367999	0.094*
H1C	1.837442	0.722679	0.268588	0.094*
C2	1.4581 (6)	0.71269 (12)	0.5685 (6)	0.0452 (10)
H2	1.552688	0.727419	0.605779	0.054*
C3	1.4661 (6)	0.69610 (12)	0.4158 (6)	0.0509 (12)
C4	1.3260 (7)	0.67413 (12)	0.3632 (8)	0.0611 (14)
H4	1.332431	0.662941	0.258148	0.073*
C5	1.1798 (7)	0.66845 (13)	0.4603 (9)	0.0681 (16)
C6	1.1710 (6)	0.68540 (13)	0.6148 (8)	0.0609 (13)
H6	1.070914	0.681825	0.683816	0.073*
C7	1.3086 (6)	0.70736 (11)	0.6665 (6)	0.0481 (11)
C8	1.1682 (7)	0.72043 (17)	0.9266 (8)	0.0724 (16)
H8A	1.194120	0.732924	1.030194	0.109*
H8B	1.153132	0.694690	0.948209	0.109*
H8C	1.059079	0.730138	0.878769	0.109*
C9[a]	1.0037 (15)	0.6470 (3)	0.4531 (15)	0.044 (2)
H9[a]	0.913318	0.649313	0.533836	0.053*
C10[a]	1.0663 (12)	0.6432 (2)	0.3626 (15)	0.0372 (18)
H10[a]	1.102255	0.635584	0.255850	0.045*
C11[a]	0.9905 (14)	0.6253 (3)	0.3251 (13)	0.0440 (19)
H11[a]	1.081149	0.621986	0.245440	0.053*
C12[a]	0.9118 (11)	0.6312 (2)	0.4280 (11)	0.0336 (17)
H12[a]	0.872784	0.638413	0.534267	0.040*
C13	0.8037 (8)	0.60526 (13)	0.3205 (10)	0.0799 (19)
C14	0.8315 (6)	0.58506 (15)	0.1778 (9)	0.0743 (16)
H14	0.943526	0.585908	0.124841	0.089*
C15	0.6971 (6)	0.56355 (13)	0.1114 (7)	0.0553 (12)
H15	0.717265	0.549595	0.015149	0.066*
C16	0.5363 (5)	0.56311 (11)	0.1883 (6)	0.0398 (9)
C17	0.5081 (7)	0.58220 (12)	0.3289 (6)	0.0531 (11)
H17	0.396460	0.581219	0.382664	0.064*
C18	0.6420 (9)	0.60287 (14)	0.3925 (8)	0.0713 (15)
H18	0.620692	0.616038	0.490824	0.086*
C19	0.3807 (6)	0.50887 (13)	0.1450 (8)	0.0618 (14)
C20	0.2143 (7)	0.49314 (13)	0.0738 (8)	0.0636 (14)
H20A	0.241611	0.481212	−0.032258	0.076*
H20B	0.128039	0.512609	0.052119	0.076*
C21	0.1346 (6)	0.46629 (13)	0.1908 (6)	0.0561 (12)
H21A	0.126468	0.477475	0.301275	0.067*
H21B	0.215776	0.445491	0.199724	0.067*
C22	−0.0493 (6)	0.45240 (14)	0.1425 (6)	0.0525 (11)
H22A	−0.134321	0.472634	0.139064	0.063*
H22B	−0.044514	0.441363	0.031555	0.063*
C23	−0.1093 (6)	0.42500 (14)	0.2666 (6)	0.0526 (12)
H23A	−0.109022	0.436320	0.377010	0.063*
H23B	−0.022160	0.405129	0.268635	0.063*
C24	−0.2915 (5)	0.40923 (12)	0.2353 (6)	0.0455 (10)
H24A	−0.378787	0.429036	0.229379	0.055*
H24B	−0.291094	0.396857	0.127275	0.055*
C25	−0.3485 (6)	0.38318 (11)	0.3654 (6)	0.0433 (10)
C26	−0.5792 (6)	0.34568 (13)	0.4621 (6)	0.0483 (11)
H26A	−0.586025	0.357113	0.572077	0.058*
H26B	−0.499205	0.324658	0.469229	0.058*
C27	−0.7599 (6)	0.33413 (14)	0.4063 (7)	0.0626 (14)
H27A	−0.809539	0.317147	0.486276	0.094*
H27B	−0.750989	0.322494	0.298297	0.094*
H27C	−0.837141	0.355220	0.398089	0.094*
O1	1.6038 (5)	0.69947 (9)	0.3073 (5)	0.0648 (10)
O2	1.3123 (4)	0.72564 (9)	0.8131 (5)	0.0599 (9)
O3	0.4910 (6)	0.49306 (11)	0.2226 (9)	0.121 (2)
O4	0.3922 (4)	0.54432 (7)	0.1182 (4)	0.0463 (8)
O5	−0.2567 (4)	0.37333 (8)	0.4797 (4)	0.0529 (8)
O6	−0.5132 (4)	0.37134 (8)	0.3401 (4)	0.0467 (7)

[a]Occupancy: 0.5.

crystallized at ambient and room temperature in four days by evaporation.

Experimental details

All hydrogen atoms were positioned geometrically and fixed in the riding model with a C–H bond distance of 0.95 Å in the riding-model approximation. Their U_{iso} values were set to be 1.2 U_{eq} of the parent atoms.

Comment

As a natural polyphenol, resveratrol was found in many plants such as pumpkin, knotweed, grapes, and peanuts [5]. It has anti-cancer, antibacterial, and antifatigue properties and has essential applications in the nutrition and food fields [6, 7]. Due to the C=C double bond having cis and trans configurations and can be interconverted under certain conditions. The hydroxyl group [8–12], benzene ring [13–16], and C=C double bond [17–20] of resveratrol can be modified to improve its biological activity and stability. Resveratrol and its derivatives have preventive effects against cancer, cardiovascular disease, neurodegenerative diseases, and inflammation. Due to their biological activities, there is growing attention to the promise of resveratrol and its derivatives as anti-aging molecules [21]. Some similar compound were synthesized and their activities were studied [22–27]. We here report a new resveratrol derivative for potential applications in food additive fields.

The figure shows the title compound. There were no significant differences observed between the two ester groups. The C=O bond lengths are 1.199(8) Å (C19=O3) and 1.215(6) Å (C25=O5), and the C–O bond lengths are 1.339(6) Å (C19–O4) and 1.336(6) Å (C25–O6), and the O=C–

O band angles are 121.5(5)° (O3=C19–O4) and 123.4(5)° (O5=C25–O6), respectively. The two aryl rings are almost in the same plane, and the dihedral angle between the C2···C7 ring and the C13···C18 ring is 6.9°. All molecules are staggered head-to-tail in the crystal, and no hydrogen bonds and π–π interactions between molecules are observed. All geometric parameters are in the expected ranges.

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