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(*E*)-1-(1,3-Benzodioxol-5-yl)-3-[4-(dimethylamino)-phenyl]prop-2-en-1-one

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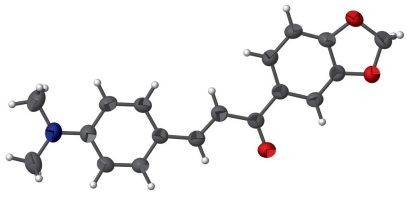
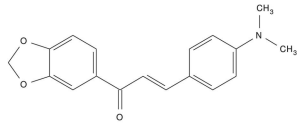
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{17}NO_3$, the olefinic double bond adopts an *E* conformation. The molecule is nearly planar as indicated by the dihedral angle of 3.11 (6)° between the benzodioxole and benzene rings. The carbonyl group lies in the plane of the olefinic double bond and the benzodioxole ring. The *trans* conformation of the C=C double bond in the central enone group is confirmed by the C=C—C—C torsion angle of −177.82 (14)°.

3D view



Chemical scheme



Structure description

Chalcones constitute the central core for the construction of a wide range of bioactive compounds (Ajay Kumar *et al.*, 2010). Chalcones and their derivatives demonstrate a wide range of biological activities, such as antioxidant, antifungal, antibacterial, cardio-protective. In view of the broad spectrum of applications associated with chalcones and as a part of our ongoing work on such molecules (Tejkiran *et al.*, 2016; Naveen *et al.*, 2016*a*), we report herein on the synthesis and crystal structure of the title compound.

The molecule (Fig. 1) is nearly planar, with a dihedral angle of 3.11 (6)° between the benzodioxole and benzene rings that are bridged by the olefinic double bond. This value is less than that reported for the dihedral angle between the aromatic rings [19.13 (15)°] in the related chalcone derivative (*E*)-3-(2,3-dichlorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (Naveen *et al.*, 2016*b*). The *trans* conformation about the C7=C8 double bond in the central enone group is confirmed by the C7=C8—C9—C10 torsion angle of −177.82 (14)°. The carbonyl group at C9 lies in the plane of the olefinic double bond and the benzodioxole ring, as indicated by the O3—C9—C8—C7 and O3—C9—C10—C16

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{17}NO_3$
M_r	295.33
Crystal system, space group	Monoclinic, $P2_1/a$
Temperature (K)	293
a, b, c (Å)	11.915 (10), 10.8405 (10), 12.184 (11)
β (°)	101.922 (8)
V (Å^3)	1539.8 (19)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.29 × 0.27 × 0.24
Data collection	
Diffractometer	Rigaku Saturn724+ CCD
Absorption correction	Multi-scan (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.975, 0.979
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7186, 3479, 2629
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.146, 1.04
No. of reflections	3479
No. of parameters	201
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.15

Computer programs: *CrystalClear SM-Expert* (Rigaku, 2011), *SHELXS97* and *SHELXL97* (Sheldrick, 208) and *Mercury* (Macrae *et al.*, 2008).

torsion angles of 2.0 (2)° and 3.7 (2)°, respectively. No classical hydrogen bonds are found in the structure.

Synthesis and crystallization

A mixture of 4-(dimethylamino)benzaldehyde (5 mmol), 1-(benzo[*d*][1,3]dioxol-5-yl)ethanone (5 mmol) and sodium hydroxide (5 mmol) in ethyl alcohol (25 ml) was stirred at room temperature for 3 h. The progress of the reaction was monitored by TLC. After the completion of the reaction, the mixture was poured into ice-cold water and kept in the refrigerator for 18 h. The solid formed was filtered, and washed with cold hydrochloric acid (5%). Single crystals suitable for X-ray diffraction studies were obtained from methyl alcohol and a few drops of acetonitrile by slow evaporation of the solvents (yield 88%, m.p. 93–94°C).

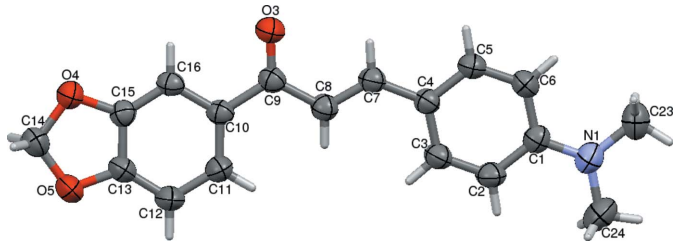


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x162029 [https://doi.org/10.1107/S2414314616020290]

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Crystal data

$C_{18}H_{17}NO_3$
M_r = 295.33
Monoclinic, $P2_1/a$
Hall symbol: -P 2yab
a = 11.915 (10) Å
b = 10.8405 (10) Å
c = 12.184 (11) Å
β = 101.922 (8)°
V = 1539.8 (19) Å^3
Z = 4
$F(000)$ = 624
D_x = 1.274 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2629 reflections
θ = 3.3–27.5°
μ = 0.09 mm^{-1}
T = 293 K
Rectangle, brown
0.29 × 0.27 × 0.24 mm

Data collection

Rigaku Saturn724+ CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 28.5714 pixels mm^{-1}
profile data from ω–scans
Absorption correction: multi-scan (NUMABS; Rigaku, 1999)
T_{min} = 0.975, T_{max} = 0.979
7186 measured reflections
3479 independent reflections
2629 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −13→15
k = −14→11
l = −15→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.146
S = 1.04
3479 reflections
201 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 0.1951P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.37832 (9)	0.20251 (12)	−0.19163 (9)	0.0595 (4)
O4	0.51384 (9)	0.08096 (12)	0.22013 (9)	0.0590 (4)
O5	0.70923 (10)	0.11039 (14)	0.26761 (9)	0.0721 (5)
N1	0.65091 (13)	0.44829 (15)	−0.73998 (12)	0.0652 (5)
C1	0.61229 (13)	0.40498 (13)	−0.64936 (12)	0.0479 (4)
C2	0.68837 (13)	0.37874 (15)	−0.54635 (13)	0.0535 (5)
C3	0.64905 (13)	0.33658 (15)	−0.45519 (12)	0.0505 (5)
C4	0.53234 (12)	0.31754 (13)	−0.45929 (11)	0.0436 (4)
C5	0.45761 (12)	0.34319 (14)	−0.56122 (12)	0.0487 (4)
C6	0.49551 (13)	0.38484 (14)	−0.65357 (12)	0.0501 (4)
C7	0.48650 (13)	0.27767 (13)	−0.36412 (12)	0.0464 (4)
C8	0.54391 (13)	0.25066 (14)	−0.26054 (12)	0.0480 (4)
C9	0.48377 (12)	0.21340 (13)	−0.17243 (12)	0.0445 (4)
C10	0.55141 (12)	0.18863 (13)	−0.05724 (11)	0.0428 (4)
C11	0.66948 (13)	0.20478 (17)	−0.02721 (13)	0.0570 (5)
C12	0.73073 (14)	0.1804 (2)	0.08137 (14)	0.0676 (6)
C13	0.66965 (13)	0.13966 (15)	0.15751 (12)	0.0528 (5)
C14	0.61240 (15)	0.07070 (16)	0.30885 (13)	0.0581 (5)
C15	0.55270 (12)	0.12316 (12)	0.12871 (11)	0.0435 (4)
C16	0.49093 (11)	0.14651 (13)	0.02312 (11)	0.0427 (4)
C23	0.57384 (18)	0.46946 (17)	−0.84656 (14)	0.0659 (6)
C24	0.7710 (2)	0.4674 (3)	−0.7342 (2)	0.0959 (10)
H2	0.76670	0.39040	−0.54050	0.0640*
H3	0.70140	0.32020	−0.38890	0.0610*
H5	0.37930	0.33160	−0.56660	0.0580*
H6	0.44280	0.39990	−0.71990	0.0600*
H7	0.40710	0.26980	−0.37650	0.0560*
H8	0.62360	0.25560	−0.24410	0.0580*
H11	0.70880	0.23260	−0.08090	0.0680*
H12	0.80970	0.19150	0.10090	0.0810*
H14A	0.60300	0.12160	0.37180	0.0700*
H14B	0.62250	−0.01420	0.33410	0.0700*
H16	0.41190	0.13500	0.00510	0.0510*
H23A	0.54370	0.39200	−0.87780	0.0990*
H23B	0.61470	0.50890	−0.89700	0.0990*
H23C	0.51190	0.52150	−0.83570	0.0990*
H24A	0.79840	0.53100	−0.68050	0.1440*
H24B	0.78310	0.49180	−0.80660	0.1440*
H24C	0.81180	0.39220	−0.71160	0.1440*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0409 (6)	0.0826 (8)	0.0527 (6)	−0.0020 (5)	0.0045 (5)	0.0061 (5)
O4	0.0485 (6)	0.0820 (8)	0.0468 (6)	−0.0035 (5)	0.0107 (5)	0.0075 (5)
O5	0.0517 (7)	0.1137 (11)	0.0457 (6)	−0.0125 (7)	−0.0020 (5)	0.0123 (6)
N1	0.0612 (9)	0.0786 (10)	0.0588 (8)	−0.0033 (7)	0.0197 (7)	0.0107 (7)
C1	0.0506 (8)	0.0465 (7)	0.0479 (8)	−0.0007 (6)	0.0133 (6)	−0.0004 (6)
C2	0.0375 (7)	0.0663 (9)	0.0561 (9)	−0.0027 (7)	0.0086 (6)	−0.0024 (7)
C3	0.0411 (7)	0.0617 (9)	0.0462 (8)	0.0008 (7)	0.0030 (6)	−0.0015 (6)
C4	0.0408 (7)	0.0475 (7)	0.0417 (7)	0.0010 (6)	0.0066 (5)	−0.0026 (5)
C5	0.0389 (7)	0.0569 (8)	0.0486 (8)	−0.0012 (6)	0.0049 (6)	0.0015 (6)
C6	0.0459 (8)	0.0570 (8)	0.0444 (7)	0.0005 (6)	0.0025 (6)	0.0032 (6)
C7	0.0421 (7)	0.0507 (8)	0.0459 (7)	−0.0004 (6)	0.0077 (6)	−0.0023 (6)
C8	0.0440 (7)	0.0542 (8)	0.0455 (7)	0.0025 (6)	0.0086 (6)	−0.0004 (6)
C9	0.0428 (7)	0.0461 (7)	0.0437 (7)	0.0006 (6)	0.0067 (6)	−0.0038 (6)
C10	0.0400 (7)	0.0438 (7)	0.0437 (7)	0.0003 (6)	0.0067 (6)	−0.0047 (5)
C11	0.0431 (8)	0.0799 (11)	0.0485 (8)	−0.0087 (7)	0.0106 (6)	0.0042 (7)
C12	0.0395 (8)	0.1049 (14)	0.0553 (9)	−0.0146 (8)	0.0024 (7)	0.0091 (9)
C13	0.0432 (8)	0.0673 (9)	0.0442 (8)	−0.0049 (7)	0.0002 (6)	0.0005 (7)
C14	0.0597 (10)	0.0676 (10)	0.0443 (8)	−0.0061 (8)	0.0045 (7)	0.0022 (7)
C15	0.0439 (7)	0.0445 (7)	0.0430 (7)	−0.0008 (6)	0.0113 (6)	−0.0034 (5)
C16	0.0362 (7)	0.0460 (7)	0.0454 (7)	0.0014 (5)	0.0070 (5)	−0.0046 (6)
C23	0.0866 (13)	0.0609 (10)	0.0524 (9)	0.0040 (9)	0.0192 (9)	0.0070 (7)
C24	0.0721 (14)	0.132 (2)	0.0898 (15)	−0.0227 (13)	0.0314 (12)	0.0242 (14)

Geometric parameters (Å, º)

O3—C9	1.235 (2)	C12—C13	1.365 (3)
O4—C14	1.427 (2)	C13—C15	1.377 (2)
O4—C15	1.370 (2)	C15—C16	1.367 (2)
O5—C13	1.364 (2)	C2—H2	0.9300
O5—C14	1.417 (3)	C3—H3	0.9300
N1—C1	1.364 (2)	C5—H5	0.9300
N1—C23	1.446 (3)	C6—H6	0.9300
N1—C24	1.433 (3)	C7—H7	0.9300
C1—C2	1.417 (2)	C8—H8	0.9300
C1—C6	1.399 (3)	C11—H11	0.9300
C2—C3	1.370 (2)	C12—H12	0.9300
C3—C4	1.397 (2)	C14—H14A	0.9700
C4—C5	1.398 (2)	C14—H14B	0.9700
C4—C7	1.446 (2)	C16—H16	0.9300
C5—C6	1.373 (2)	C23—H23A	0.9600
C7—C8	1.338 (2)	C23—H23B	0.9600
C8—C9	1.465 (2)	C23—H23C	0.9600
C9—C10	1.491 (2)	C24—H24A	0.9600
C10—C11	1.390 (2)	C24—H24B	0.9600
C10—C16	1.406 (2)	C24—H24C	0.9600

C11—C12	1.398 (3)		
C14—O4—C15	106.17 (12)	C3—C2—H2	119.00
C13—O5—C14	106.13 (12)	C2—C3—H3	119.00
C1—N1—C23	121.59 (15)	C4—C3—H3	119.00
C1—N1—C24	120.68 (16)	C4—C5—H5	119.00
C23—N1—C24	117.63 (16)	C6—C5—H5	119.00
N1—C1—C2	121.66 (15)	C1—C6—H6	120.00
N1—C1—C6	121.55 (14)	C5—C6—H6	120.00
C2—C1—C6	116.78 (13)	C4—C7—H7	116.00
C1—C2—C3	121.45 (14)	C8—C7—H7	116.00
C2—C3—C4	121.67 (14)	C7—C8—H8	119.00
C3—C4—C5	116.68 (13)	C9—C8—H8	119.00
C3—C4—C7	123.62 (13)	C10—C11—H11	119.00
C5—C4—C7	119.66 (13)	C12—C11—H11	119.00
C4—C5—C6	122.45 (14)	C11—C12—H12	121.00
C1—C6—C5	120.96 (14)	C13—C12—H12	121.00
C4—C7—C8	128.14 (15)	O4—C14—H14A	110.00
C7—C8—C9	121.29 (14)	O4—C14—H14B	110.00
O3—C9—C8	121.32 (13)	O5—C14—H14A	110.00
O3—C9—C10	119.46 (13)	O5—C14—H14B	110.00
C8—C9—C10	119.22 (13)	H14A—C14—H14B	108.00
C9—C10—C11	123.09 (13)	C10—C16—H16	121.00
C9—C10—C16	117.30 (13)	C15—C16—H16	121.00
C11—C10—C16	119.61 (13)	N1—C23—H23A	109.00
C10—C11—C12	121.85 (15)	N1—C23—H23B	110.00
C11—C12—C13	117.19 (15)	N1—C23—H23C	109.00
O5—C13—C12	128.23 (15)	H23A—C23—H23B	109.00
O5—C13—C15	110.28 (13)	H23A—C23—H23C	109.00
C12—C13—C15	121.50 (14)	H23B—C23—H23C	109.00
O4—C14—O5	108.10 (12)	N1—C24—H24A	109.00
O4—C15—C13	109.30 (12)	N1—C24—H24B	109.00
O4—C15—C16	128.32 (13)	N1—C24—H24C	109.00
C13—C15—C16	122.38 (13)	H24A—C24—H24B	110.00
C10—C16—C15	117.48 (13)	H24A—C24—H24C	109.00
C1—C2—H2	119.00	H24B—C24—H24C	110.00
C15—O4—C14—O5	1.21 (17)	C4—C5—C6—C1	−0.7 (2)
C14—O4—C15—C13	−0.31 (16)	C4—C7—C8—C9	178.89 (14)
C14—O4—C15—C16	179.25 (14)	C7—C8—C9—O3	2.0 (2)
C14—O5—C13—C12	−178.77 (18)	C7—C8—C9—C10	−177.82 (14)
C14—O5—C13—C15	1.48 (18)	O3—C9—C10—C11	−176.62 (15)
C13—O5—C14—O4	−1.65 (18)	O3—C9—C10—C16	3.7 (2)
C23—N1—C1—C2	177.02 (15)	C8—C9—C10—C11	3.2 (2)
C24—N1—C1—C2	0.8 (3)	C8—C9—C10—C16	−176.56 (13)
C23—N1—C1—C6	−3.3 (2)	C9—C10—C11—C12	−179.77 (16)
C24—N1—C1—C6	−179.52 (19)	C16—C10—C11—C12	−0.1 (3)
N1—C1—C2—C3	179.25 (15)	C9—C10—C16—C15	179.72 (13)

C6—C1—C2—C3	−0.5 (2)	C11—C10—C16—C15	0.0 (2)
N1—C1—C6—C5	−178.90 (15)	C10—C11—C12—C13	0.0 (3)
C2—C1—C6—C5	0.8 (2)	C11—C12—C13—O5	−179.69 (17)
C1—C2—C3—C4	−0.1 (3)	C11—C12—C13—C15	0.0 (3)
C2—C3—C4—C5	0.2 (2)	O5—C13—C15—O4	−0.75 (18)
C2—C3—C4—C7	−177.57 (15)	O5—C13—C15—C16	179.66 (14)
C3—C4—C5—C6	0.1 (2)	C12—C13—C15—O4	179.48 (16)
C7—C4—C5—C6	178.02 (14)	C12—C13—C15—C16	−0.1 (2)
C3—C4—C7—C8	−1.3 (2)	O4—C15—C16—C10	−179.42 (14)
C5—C4—C7—C8	−179.10 (15)	C13—C15—C16—C10	0.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O3	0.93	2.46	2.804 (3)	102