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p-Cresyl cinnamate

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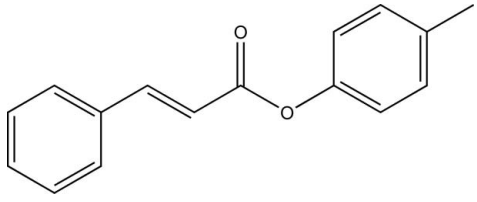
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.073; wR factor = 0.180; data-to-parameter ratio = 17.2.

In the crystal structure of the title compound [4-methylphenyl (*E*)-3-phenylpropenoate], $C_{16}H_{14}O_2$, the benzene ring of the cinnamoyl group is slightly distorted due to conjugation with the double bond. The mean plane of the cinnamoyl group forms a dihedral angle of 61.1 (1)° with the plane of the cresyl group.

Related literature

Several structures of cinnamate esters with simple aromatic alcohols have been reported previously: coumaryl cinnamate (Yang *et al.*, 2006), pentafluorophenyl cinnamate (Andrade *et al.*, 2006) and 2-chlorophenyl cinnamate (Nilofar Nissa *et al.*, 2004). For a discussion of ring deformations induced by substitution in benzene derivatives, see: Domenicano *et al.* (1975).



Experimental

Crystal data

$C_{16}H_{14}O_2$
M_r = 238.27
Monoclinic, $C2/c$
a = 20.236 (3) Å
b = 7.5613 (11) Å
c = 17.379 (3) Å
β = 102.573 (12)°
V = 2595.5 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.40 × 0.24 × 0.23 mm

Data collection

Oxford Diffraction Xcalibur CCD diffractometer
Absorption correction: none
9394 measured reflections
2816 independent reflections
2173 reflections with $I > 2\sigma(I)$
R_{int} = 0.076

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.180
S = 1.13
2816 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2242).

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supplementary materials

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Comment

In the title compound (Fig. 1), the majority of bond lengths and angles have normal values, in accord with those of related compounds. The geometry of the phenyl ring C4–C9 is mildly distorted, with the endocyclic angle C5—C4—C9 = 117.7 (2)° and the aromatic C—C bonds adjacent to C4 somewhat longer than neighbouring ones. Also, the C3—C4 bond (1.461 (3) Å) is somewhat shorter than the reported average for C(aromatic)—Csp^2 bonds (1.483 Å). These distortions can be attributed to hybridization and conjugation effects (Domenicano *et al.*, 1975). The cinnamoyl group is almost perfectly planar and forms an angle of 61.6 (1)° with the cresyl ring.

Cresyl groups participate in C—H···π intermolecular contacts (C15···C13^{i} = 3.613 (5) Å, C15—H15···C13 = 148.4°; symmetry code: (i) 1/2 − *x*, −1/2 + *y*, 1/2 − *z*), while the cinnamoyl groups do not participate in any notable intermolecular interactions.

Experimental

The title compound was prepared unintentionally while attempting to isolate a 1,3,3'-triketone containing a cinnamoyl group. To an isooctane solution containing sodium dipivaloilmethanate (0.15 g in 10 ml), a solution of cinnamoyl chloride (0.18 g) in isooctane (8 ml) was added. The precipitate of sodium chloride was filtered off and a solution of *p*-cresol (0.1 g) in dichloromethane (15 ml) was added to the clear solution. Colourless crystals were obtained on standing at room temperature overnight.

Refinement

H atoms were placed geometrically and included in the refinement in the riding-model approximation, with C—H distances of 0.93 or 0.96 Å and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Figures

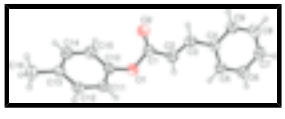

Fig. 1. The molecular structure of the title compound with displacement ellipsoids shown at 30% probability for non-H atoms.

4-methylphenyl (*E*)-3-phenylpropenoate

Crystal data

$C_{16}H_{14}O_2$	F_{000} = 1008
M_r = 238.27	D_x = 1.22 Mg m^{-3}

Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1344 reflections
a = 20.236 (3) Å	θ = 4.6–52.0º
b = 7.5613 (11) Å	μ = 0.08 mm^{-1}
c = 17.379 (3) Å	*T* = 295 (2) K
β = 102.573 (12)º	Bipyramidal, colourless
V = 2595.5 (7) $Å^3$	0.40 × 0.24 × 0.23 mm
Z = 8	

Data collection

Oxford Diffraction Xcalibur CCD diffractometer	2173 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.076
Monochromator: graphite	θ_{max} = 27.0º
T = 295(2) K	θ_{min} = 4.1º
ω scans	*h* = −25→25
Absorption correction: none	*k* = −9→9
9394 measured reflections	*l* = −22→21
2816 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0682P)^2 + 1.203P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.073	$(\Delta/\sigma)_{max}$ = 0.042
$wR(F^2)$ = 0.180	$\Delta\rho_{max}$ = 0.17 e $Å^{-3}$
S = 1.13	$\Delta\rho_{min}$ = −0.19 e $Å^{-3}$
2816 reflections	Extinction correction: none
164 parameters	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.17548 (8)	0.7483 (2)	0.39340 (10)	0.0734 (5)
C10	0.23187 (10)	0.7149 (3)	0.36090 (12)	0.0548 (5)
C2	0.06545 (11)	0.7133 (3)	0.40768 (13)	0.0624 (6)
H2	0.0791	0.7782	0.4539	0.075*

C4	−0.05010 (10)	0.6773 (3)	0.43304 (12)	0.0543 (5)
C13	0.35019 (11)	0.6650 (3)	0.30803 (12)	0.0573 (5)
C1	0.11498 (10)	0.6761 (3)	0.35991 (12)	0.0580 (5)
C11	0.28404 (11)	0.6212 (3)	0.40606 (12)	0.0583 (5)
H11	0.2801	0.575	0.4544	0.07*
C12	0.34259 (10)	0.5961 (3)	0.37904 (12)	0.0578 (5)
H12	0.3778	0.5311	0.4095	0.069*
C3	0.00252 (11)	0.6586 (3)	0.38786 (13)	0.0591 (5)
H3	−0.01	0.6014	0.3395	0.071*
C5	−0.03804 (11)	0.7590 (3)	0.50668 (13)	0.0645 (6)
H5	0.0046	0.8053	0.528	0.077*
O2	0.10590 (8)	0.5906 (3)	0.30051 (10)	0.0839 (6)
C9	−0.11400 (11)	0.6114 (3)	0.40350 (14)	0.0670 (6)
H9	−0.1234	0.5574	0.3543	0.08*
C14	0.29647 (12)	0.7582 (3)	0.26392 (14)	0.0673 (6)
H14	0.3003	0.8057	0.2157	0.081*
C15	0.23739 (12)	0.7827 (3)	0.28933 (14)	0.0676 (6)
H15	0.2015	0.8445	0.2584	0.081*
C6	−0.08837 (13)	0.7720 (4)	0.54816 (14)	0.0716 (7)
H6	−0.0797	0.8274	0.5971	0.086*
C7	−0.15159 (12)	0.7033 (4)	0.51757 (16)	0.0729 (7)
H7	−0.1854	0.711	0.546	0.087*
C8	−0.16446 (12)	0.6238 (4)	0.44532 (17)	0.0756 (7)
H8	−0.2072	0.5781	0.4243	0.091*
C16	0.41478 (13)	0.6383 (5)	0.27968 (17)	0.0884 (9)
H16A	0.4056	0.5687	0.2323	0.133*
H16B	0.4472	0.578	0.3196	0.133*
H16C	0.4327	0.7511	0.2691	0.133*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0581 (9)	0.0885 (13)	0.0752 (10)	−0.0037 (8)	0.0182 (7)	−0.0242 (9)
C10	0.0516 (11)	0.0547 (13)	0.0583 (12)	−0.0037 (9)	0.0126 (9)	−0.0076 (9)
C2	0.0596 (13)	0.0647 (15)	0.0621 (13)	0.0051 (11)	0.0114 (10)	−0.0103 (11)
C4	0.0533 (11)	0.0498 (11)	0.0590 (11)	0.0069 (9)	0.0107 (9)	0.0021 (9)
C13	0.0594 (12)	0.0577 (13)	0.0553 (11)	−0.0116 (10)	0.0134 (9)	−0.0050 (10)
C1	0.0545 (12)	0.0612 (13)	0.0582 (12)	0.0062 (10)	0.0117 (9)	−0.0012 (10)
C11	0.0648 (12)	0.0629 (14)	0.0466 (10)	−0.0049 (11)	0.0109 (9)	0.0023 (9)
C12	0.0570 (12)	0.0581 (13)	0.0551 (11)	0.0022 (10)	0.0049 (9)	0.0026 (10)
C3	0.0617 (12)	0.0575 (13)	0.0568 (12)	0.0065 (10)	0.0103 (9)	−0.0050 (10)
C5	0.0583 (12)	0.0745 (16)	0.0594 (13)	0.0025 (11)	0.0101 (10)	−0.0017 (11)
O2	0.0670 (10)	0.1127 (16)	0.0753 (11)	−0.0096 (10)	0.0225 (8)	−0.0308 (11)
C9	0.0647 (13)	0.0609 (14)	0.0756 (14)	−0.0021 (11)	0.0159 (11)	−0.0122 (12)
C14	0.0752 (15)	0.0693 (15)	0.0579 (12)	−0.0102 (12)	0.0155 (11)	0.0138 (11)
C15	0.0681 (14)	0.0624 (15)	0.0677 (14)	0.0069 (11)	0.0047 (11)	0.0150 (11)
C6	0.0765 (15)	0.0844 (18)	0.0564 (13)	0.0070 (13)	0.0198 (11)	0.0014 (12)
C7	0.0669 (14)	0.0771 (18)	0.0813 (16)	0.0089 (13)	0.0307 (12)	0.0124 (13)

C8	0.0603 (13)	0.0706 (17)	0.0969 (18)	−0.0080 (12)	0.0190 (13)	−0.0069 (14)
C16	0.0716 (16)	0.113 (2)	0.0879 (18)	−0.0145 (16)	0.0338 (14)	−0.0107 (16)

Geometric parameters (Å, °)

O1—C1	1.351 (3)	C3—H3	0.93
O1—C10	1.402 (2)	C5—C6	1.374 (3)
C10—C11	1.368 (3)	C5—H5	0.93
C10—C15	1.372 (3)	C9—C8	1.379 (3)
C2—C3	1.312 (3)	C9—H9	0.93
C2—C1	1.461 (3)	C14—C15	1.374 (3)
C2—H2	0.93	C14—H14	0.93
C4—C9	1.376 (3)	C15—H15	0.93
C4—C5	1.394 (3)	C6—C7	1.376 (4)
C4—C3	1.461 (3)	C6—H6	0.93
C13—C12	1.379 (3)	C7—C8	1.365 (4)
C13—C14	1.380 (3)	C7—H7	0.93
C13—C16	1.508 (3)	C8—H8	0.93
C1—O2	1.198 (3)	C16—H16A	0.96
C11—C12	1.379 (3)	C16—H16B	0.96
C11—H11	0.93	C16—H16C	0.96
C12—H12	0.93		
C1—O1—C10	119.64 (17)	C6—C5—H5	119.6
C11—C10—C15	120.6 (2)	C4—C5—H5	119.6
C11—C10—O1	117.14 (19)	C4—C9—C8	121.5 (2)
C15—C10—O1	122.2 (2)	C4—C9—H9	119.3
C3—C2—C1	122.5 (2)	C8—C9—H9	119.3
C3—C2—H2	118.8	C15—C14—C13	121.7 (2)
C1—C2—H2	118.8	C15—C14—H14	119.1
C9—C4—C5	117.7 (2)	C13—C14—H14	119.1
C9—C4—C3	120.0 (2)	C10—C15—C14	119.3 (2)
C5—C4—C3	122.26 (19)	C10—C15—H15	120.3
C12—C13—C14	117.5 (2)	C14—C15—H15	120.3
C12—C13—C16	121.0 (2)	C5—C6—C7	120.2 (2)
C14—C13—C16	121.4 (2)	C5—C6—H6	119.9
O2—C1—O1	123.0 (2)	C7—C6—H6	119.9
O2—C1—C2	126.7 (2)	C8—C7—C6	119.8 (2)
O1—C1—C2	110.30 (18)	C8—C7—H7	120.1
C10—C11—C12	119.25 (19)	C6—C7—H7	120.1
C10—C11—H11	120.4	C7—C8—C9	120.0 (2)
C12—C11—H11	120.4	C7—C8—H8	120
C13—C12—C11	121.6 (2)	C9—C8—H8	120
C13—C12—H12	119.2	C13—C16—H16A	109.5
C11—C12—H12	119.2	C13—C16—H16B	109.5
C2—C3—C4	127.4 (2)	H16A—C16—H16B	109.5
C2—C3—H3	116.3	C13—C16—H16C	109.5
C4—C3—H3	116.3	H16A—C16—H16C	109.5
C6—C5—C4	120.8 (2)	H16B—C16—H16C	109.5

Fig. 1