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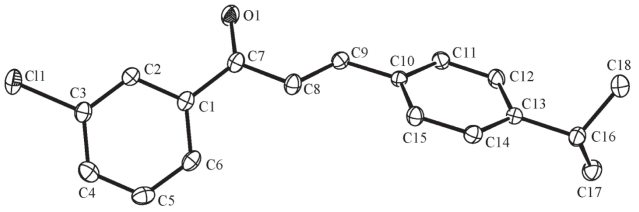
Crystal structure of (*E*)-3-(4-*tert*-butyl)phenyl)-1-(3-chlorophenyl)prop-2-en-1-one, $C_{18}H_{17}ClO$



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Abstract

$C_{18}H_{17}ClO$, monoclinic, $P2_1/c$ (No. 14), $a = 5.9172(3)$ Å, $b = 7.5758(6)$ Å, $c = 33.1334(16)$ Å, $\beta = 93.666(5)°$, $V = 1482.2(16)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0453$, $wR_{ref}(F^2) = 0.1116$, $T = 180$ K.

CCDC no.: 1267/4371

Table 1: Data collection and handling.

Crystal:	Colorless, blocks, size 0.1×0.2×0.2 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	2.50 cm^{-1}
Diffractometer, scan mode:	SuperNova, Dual, Cu at zero, Atlas, ω scans
$2\theta_{max}$:	52.03°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6863, 2912
$N(param)_{refined}$:	183
Programs:	SUPERFLIP, J. APPL. CRYST. (2007) 40, 786–790

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Table 2: Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	4*e*	0.2869	0.2776	0.4122	0.032
H(4)	4*e*	0.764	0.5148	0.3485	0.043
H(5)	4*e*	1.0059	0.5298	0.4068	0.045
H(6)	4*e*	0.8946	0.4143	0.4674	0.038
H(8)	4*e*	0.8206	0.1845	0.5088	0.039
H(9)	4*e*	0.4717	0.2132	0.5609	0.033
H(11)	4*e*	0.5821	0.2153	0.6325	0.036
H(12)	4*e*	0.8330	0.1471	0.687	0.038
H(14)	4*e*	1.2748	−0.0451	0.6106	0.034
H(15)	4*e*	1.031	0.0303	0.5557	0.034
H(16)	4*e*	1.3823	−0.0575	0.6792	0.04
H(17A)	4*e*	1.1949	0.221	0.725	0.061
H(17B)	4*e*	1.3996	0.244	0.6961	0.061
H(17C)	4*e*	1.4332	0.1278	0.7364	0.061
H(18A)	4*e*	1.0078	−0.084	0.7292	0.086
H(18B)	4*e*	1.2544	−0.1629	0.7407	0.086
H(18C)	4*e*	1.1032	−0.2424	0.7032	0.086

Source of material

The title compound α,β-unsaturated was prepared according to the literature method [3–5]. 4-Iso-propylbenzaldehyde (1.5 g, 10 mmol), 3′-chloroacetophenone (1.56 g, 10 mmol) were dissolved in minimum amount of alcohol. A sodium hydroxide solution (20 mmol) was added slowly and the mixture stirred at room temperature for 4 hours until the entire mixture becomes very cloudy. The mixture was left overnight in refrigerator. The separated solid was filtered, washed with water and dried, then recrystallized from ethanol as colorless needles, the title compound was gotten. The title compound was dissolved in methanol at room temperature. Colorless blocks were obtained through slow evaporation after two weeks.

Experimental details

All H atoms were placed at calculated positions.

Discussion

1-(3-Chlorophenyl)-3-(4-isopropylphenyl)prop-2-en-1-one and its derivatives are important antimicrobial intermediates [6, 7]. The crystal structures of some similar chalcone

Table 3: Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*e*	0.5801(3)	0.3341(3)	0.44599(5)	0.0269(9)	0.0239(12)	0.0279(9)	0.0081(8)	−0.0024(8)	−0.0037(8)
C(2)	4*e*	0.4339(3)	0.3273(3)	0.41119(5)	0.0248(9)	0.0247(12)	0.0301(9)	0.0044(8)	0.0004(8)	−0.0023(8)
C(3)	4*e*	0.5057(3)	0.3934(3)	0.37552(5)	0.0323(10)	0.0287(12)	0.0286(9)	0.0066(9)	−0.0023(8)	−0.0005(9)
C(4)	4*e*	0.7177(3)	0.4691(3)	0.37340(6)	0.0395(11)	0.0275(13)	0.0399(11)	0.0066(9)	0.0078(9)	0.0085(10)
C(5)	4*e*	0.8607(3)	0.4772(3)	0.40783(6)	0.0282(10)	0.0301(14)	0.0530(13)	0.0003(9)	0.0018(9)	0.0017(10)
C(6)	4*e*	0.7941(3)	0.4095(3)	0.44386(6)	0.0294(10)	0.0274(13)	0.0377(10)	0.0057(9)	−0.0073(8)	−0.0045(9)
C(7)	4*e*	0.4980(3)	0.2661(3)	0.48471(5)	0.0309(10)	0.0298(13)	0.0274(9)	0.0058(9)	−0.0025(8)	−0.0062(9)
C(8)	4*e*	0.6712(3)	0.2083(3)	0.51621(5)	0.0302(10)	0.0367(14)	0.0292(10)	0.0090(9)	−0.0011(8)	−0.0005(9)
C(9)	4*e*	0.6230(3)	0.1889(3)	0.55459(5)	0.0262(9)	0.0263(12)	0.0380(10)	0.0015(8)	−0.0001(8)	−0.0012(9)
C(10)	4*e*	0.7812(3)	0.1336(3)	0.58823(5)	0.0247(9)	0.0231(12)	0.0265(9)	−0.0026(8)	−0.0002(7)	0.0009(8)
C(11)	4*e*	0.7249(3)	0.1646(3)	0.62773(5)	0.0252(9)	0.0342(12)	0.0310(9)	0.0052(8)	0.0058(8)	0.0034(9)
C(12)	4*e*	0.8741(3)	0.1226(3)	0.66032(5)	0.0321(10)	0.0413(14)	0.0232(9)	0.0038(9)	0.0056(8)	0.0009(9)
C(13)	4*e*	1.0822(3)	0.0456(3)	0.65462(5)	0.0247(9)	0.0283(12)	0.0261(9)	−0.0014(8)	0.00003(8)	0.0029(8)
C(14)	4*e*	1.1349(3)	0.0105(3)	0.61517(5)	0.0258(9)	0.0272(12)	0.0325(10)	0.0037(8)	0.003(8)	0.0004(9)
C(15)	4*e*	0.9891(3)	0.0544(3)	0.58240(5)	0.0318(10)	0.0313(13)	0.0230(9)	0.0024(9)	0.002(8)	−0.00025(9)
C(16)	4*e*	1.2461(3)	-0.0016(3)	0.69027(5)	0.0282(9)	0.0420(14)	0.0295(10)	0.0037(9)	−0.001(8)	0.00047(9)
C(17)	4*e*	1.3256(3)	0.1626(3)	0.71406(6)	0.0380(11)	0.0527(17)	0.0314(10)	−0.0013(10)	−0.0008(9)	−0.00029(10)
C(18)	4*e*	1.1438(4)	-0.1346(4)	0.71835(7)	0.0487(13)	0.0067(2)	0.0552(14)	−0.01(13)	−0.0127(11)	0.00312(14)
Cl(1)	4*e*	0.32640(8)	0.38231(8)	0.33164(2)	0.0488(3)	0.0545(4)	0.0281(3)	0.0066(3)	−0.0082(2)	0.00012(2)
O(1)	4*e*	0.2954(2)	0.2590(2)	0.48992(4)	0.0286(7)	0.0595(12)	0.0322(7)	0.0059(7)	−0.0004(6)	0.00018(7)

derivatives have been reported [8, 9]. The molecule consists of a (4-*tert*-butyl)phenyl and a 3-chlorophenyl moiety, both rings are connected by a propenone linker. No significant hydrogen bonding or π-π stacking interactions are found in the crystal structure.

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