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(2*E*)-3-(4-Chlorophenyl)-1-[4-(methylsulfanyl)phenyl]prop-2-en-1-one

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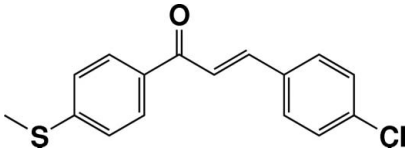
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.077; data-to-parameter ratio = 26.0.

In the title molecule, $C_{16}H_{13}ClOS$, the dihedral angle between the two benzene rings is 51.0 (1)°.

Related literature

For the uses of chalcones, see: Dhar (1981). For related crystal structures, see: Rabinovich & Shakked (1974); Ravishankar *et al.* (2005); Schmalle *et al.* (1990).



Experimental

Crystal data

$C_{16}H_{13}ClOS$
M_r = 288.78
Monoclinic, $P2_1/c$
a = 16.515 (1) Å
b = 14.3026 (9) Å
c = 5.7280 (3) Å
β = 91.284 (5)°
V = 1352.66 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 200 (2) K
0.46 × 0.37 × 0.29 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.829, T_{max} = 1.000 (expected range = 0.733–0.884)
12209 measured reflections
4494 independent reflections
2386 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.077
S = 0.86
4494 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

RJB acknowledges the NSF–MRI program for funding to purchase the X-ray CCD diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2045).

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supplementary materials

Acta Cryst. (2007). E**63**, o4716 [**doi:10.1107/S1600536807056656**]

(2*E*)-3-(4-Chlorophenyl)-1-[4-(methylsulfanyl)phenyl]prop-2-en-1-one

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Comment

Many patents have appeared in literature describing the usefulness of Chalcones and their derivatives. Their diverse applications such as artificial sweeteners, stabilizers against heat and visible light, color photography, scintillators, polymerization catalysts, fluorescent lightning agents and as brightening agents are well studied and documented (Dhar, 1981). The title material is used as an intermediate to prepare the corresponding pyrazole derivatives which have shown better antiinflamatory and analgesic activities. In the title molecule, $C_{16}H_{13}ClOS$, Fig.1, the dihedral angle between the two phenyl rings is 51.0 (1)°. The presence of a methylsulfanylphenyl group in the title molecule causes the 4-chlorophenyl group to twist away from each other. There are no classical hydrogen bonds found in the structure. In similar structures like 4,4'-Dimethylchalcone (Rabinovich & Shakked, 1974), 2',6'-Dihydroxy-4,4'-dimethoxychalcone (Schmalle *et al.*, 1990) and 1-(4-Chlorophenyl)-3-(4-hydroxyphenyl) prop-2-en-1-one(Ravishankar *et al.*, 2005), the dihedral angle between the two phenyl rings are 48.6°, 13.1 (4)° and 26.1 (1)° respectively.

Experimental

4-Chlororobenzaldehyde (2.5 g, 0.02 mol) in ethanol is mixed with 4-methylthio acetophenone (2.80 g, 0.02 mol) in 50 ml e thanol and the mixture was treated with 10 ml of 10% NaOH solution at 283 K and stirred for 8 h. The precipitate obtained was filtered, washed with ethanol and dried. Pale yellow rods of the title compound were grown from toluene by slow evaporation. The yield of the isolated product was 3.5 g (60%)

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95–0.98Å and U_{iso}=1.2 to 1.5 times U_{eq}(C).

Figures

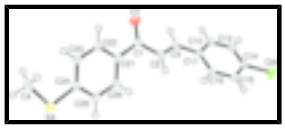


Fig. 1. The molecular structure of the title compound with the atomic numbering and 50% probability displacement ellipsoids. H atoms are shown shown as small spheres of arbitrary radius.

(2E)-3-(4-Chlorophenyl)-1-[4-(methylsulfanyl)phenyl]prop-2-en-1-one

Crystal data

$C_{16}H_{13}ClOS$	F_{000} = 600
M_r = 288.78	D_x = 1.418 Mg m^{-3}

Monoclinic, $P2_1/c$	Melting point: 444(1) K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 16.515 (1) Å	Cell parameters from 4494 reflections
b = 14.3026 (9) Å	θ = 4.5–32.6º
c = 5.7280 (3) Å	μ = 0.42 mm^{-1}
β = 91.284 (5)º	T = 200 (2) K
V = 1352.66 (14) Å^3	Prism, colourless
Z = 4	0.46 × 0.37 × 0.29 mm

Data collection

Oxford Diffraction Gemini diffractometer	4494 independent reflections
Radiation source: fine-focus sealed tube	2386 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 200(2) K	θ_{max} = 32.6º
φ and ω scans	θ_{min} = 4.5º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	h = −24→22
T_{min} = 0.829, T_{max} = 1.000	k = −21→21
12209 measured reflections	l = −8→7

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.035	H-atom parameters constrained
$wR(F^2)$ = 0.077	$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.86	$(\Delta/\sigma)_{max}$ = <0.001
4494 reflections	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
173 parameters	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness 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 threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl4	0.97354 (2)	0.13561 (3)	−0.14833 (6)	0.0456 (1)
S4	0.18062 (2)	0.10519 (3)	0.17298 (6)	0.0317 (1)
O1	0.54563 (6)	0.14122 (7)	0.71632 (15)	0.0382 (3)
C1	0.52954 (8)	0.13336 (9)	0.5078 (2)	0.0266 (4)
C2	0.59470 (8)	0.13108 (9)	0.3341 (2)	0.0276 (4)
C3	0.66980 (8)	0.10839 (9)	0.3972 (2)	0.0245 (4)
C4	0.12122 (9)	0.15828 (11)	0.3950 (3)	0.0417 (5)
C11	0.74201 (8)	0.11142 (8)	0.2543 (2)	0.0225 (4)
C12	0.81511 (8)	0.07634 (9)	0.3441 (2)	0.0264 (4)
C13	0.88615 (8)	0.08273 (9)	0.2223 (2)	0.0293 (4)
C14	0.88454 (8)	0.12614 (9)	0.0085 (2)	0.0269 (4)
C15	0.81354 (8)	0.16220 (9)	−0.0877 (2)	0.0263 (4)
C16	0.74260 (8)	0.15401 (8)	0.0342 (2)	0.0246 (4)
C21	0.44370 (8)	0.12768 (8)	0.4239 (2)	0.0232 (4)
C22	0.38269 (8)	0.15922 (8)	0.5672 (2)	0.0255 (4)
C23	0.30208 (8)	0.15462 (8)	0.4988 (2)	0.0264 (4)
C24	0.28069 (8)	0.11603 (8)	0.2817 (2)	0.0230 (4)
C25	0.34163 (8)	0.08362 (9)	0.1382 (2)	0.0264 (4)
C26	0.42171 (8)	0.09072 (9)	0.2052 (2)	0.0274 (4)
H2	0.58245	0.14608	0.17562	0.0331*
H3	0.67768	0.08772	0.55367	0.0294*
H4A	0.06385	0.15646	0.34764	0.0626*
H4B	0.12909	0.12401	0.54194	0.0626*
H4C	0.13824	0.22339	0.41688	0.0626*
H12	0.81606	0.04723	0.49317	0.0317*
H13	0.93518	0.05757	0.28528	0.0351*
H15	0.81356	0.19222	−0.23563	0.0315*
H16	0.69352	0.17762	−0.03236	0.0296*
H22	0.39678	0.18459	0.71588	0.0306*
H23	0.26141	0.17753	0.59856	0.0317*
H25	0.32756	0.05620	−0.00824	0.0316*
H26	0.46250	0.07040	0.10248	0.0328*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl4	0.0292 (2)	0.0657 (3)	0.0423 (2)	−0.0028 (2)	0.0115 (2)	0.0008 (2)
S4	0.0282 (2)	0.0334 (2)	0.0331 (2)	−0.0029 (2)	−0.0041 (1)	−0.0008 (2)
O1	0.0310 (6)	0.0587 (7)	0.0249 (5)	0.0038 (5)	−0.0013 (4)	−0.0022 (4)
C1	0.0282 (8)	0.0263 (7)	0.0253 (7)	0.0026 (6)	0.0019 (5)	0.0014 (6)
C2	0.0268 (7)	0.0326 (7)	0.0235 (7)	−0.0006 (6)	0.0012 (5)	0.0019 (6)
C3	0.0275 (7)	0.0243 (7)	0.0218 (6)	−0.0005 (6)	0.0023 (5)	0.0002 (5)
C4	0.0252 (8)	0.0474 (9)	0.0526 (9)	0.0041 (7)	0.0014 (6)	−0.0073 (7)
C11	0.0247 (7)	0.0201 (6)	0.0225 (6)	−0.0015 (5)	−0.0011 (5)	−0.0026 (5)

C12	0.0296 (7)	0.0263 (7)	0.0232 (6)	0.0014 (6)	−0.0024 (5)	0.0017 (5)
C13	0.0242 (7)	0.0339 (8)	0.0295 (7)	0.0033 (6)	−0.0031 (5)	−0.0013 (6)
C14	0.0244 (7)	0.0282 (7)	0.0282 (7)	−0.0042 (6)	0.0041 (5)	−0.0060 (6)
C15	0.0316 (8)	0.0267 (7)	0.0205 (6)	−0.0014 (6)	0.0008 (5)	0.0002 (5)
C16	0.0242 (7)	0.0262 (7)	0.0234 (7)	0.0018 (6)	−0.0023 (5)	−0.0020 (5)
C21	0.0243 (7)	0.0220 (7)	0.0235 (6)	0.0003 (5)	0.0043 (5)	0.0020 (5)
C22	0.0287 (7)	0.0274 (7)	0.0204 (6)	−0.0009 (6)	0.0011 (5)	−0.0008 (5)
C23	0.0260 (7)	0.0275 (7)	0.0260 (7)	0.0011 (6)	0.0060 (5)	−0.0016 (5)
C24	0.0267 (7)	0.0188 (6)	0.0236 (6)	−0.0023 (5)	−0.0002 (5)	0.0035 (5)
C25	0.0316 (8)	0.0271 (7)	0.0204 (6)	−0.0031 (6)	0.0016 (5)	−0.0015 (5)
C26	0.0300 (8)	0.0279 (7)	0.0245 (7)	0.0011 (6)	0.0085 (5)	−0.0009 (6)

Geometric parameters (Å, °)

Cl4—C14	1.7450 (13)	C23—C24	1.3986 (16)
S4—C4	1.7922 (17)	C24—C25	1.3930 (18)
S4—C24	1.7598 (13)	C25—C26	1.3726 (19)
O1—C1	1.2230 (14)	C2—H2	0.9500
C1—C2	1.4822 (18)	C3—H3	0.9500
C1—C21	1.4889 (18)	C4—H4A	0.9800
C2—C3	1.3244 (19)	C4—H4B	0.9800
C3—C11	1.4621 (18)	C4—H4C	0.9800
C11—C12	1.3950 (18)	C12—H12	0.9500
C11—C16	1.4004 (16)	C13—H13	0.9500
C12—C13	1.3814 (18)	C15—H15	0.9500
C13—C14	1.3728 (17)	C16—H16	0.9500
C14—C15	1.3841 (18)	C22—H22	0.9500
C15—C16	1.3822 (18)	C23—H23	0.9500
C21—C22	1.3891 (18)	C25—H25	0.9500
C21—C26	1.4001 (17)	C26—H26	0.9500
C22—C23	1.3809 (19)		
C4—S4—C24	103.66 (7)	C1—C2—H2	120.00
O1—C1—C2	120.83 (12)	C3—C2—H2	120.00
O1—C1—C21	120.31 (11)	C2—C3—H3	116.00
C2—C1—C21	118.85 (10)	C11—C3—H3	116.00
C1—C2—C3	120.78 (11)	S4—C4—H4A	109.00
C2—C3—C11	127.63 (11)	S4—C4—H4B	109.00
C3—C11—C12	119.53 (11)	S4—C4—H4C	109.00
C3—C11—C16	122.62 (11)	H4A—C4—H4B	109.00
C12—C11—C16	117.71 (12)	H4A—C4—H4C	109.00
C11—C12—C13	121.86 (11)	H4B—C4—H4C	109.00
C12—C13—C14	118.74 (12)	C11—C12—H12	119.00
Cl4—C14—C13	119.65 (10)	C13—C12—H12	119.00
Cl4—C14—C15	118.82 (9)	C12—C13—H13	121.00
C13—C14—C15	121.53 (12)	C14—C13—H13	121.00
C14—C15—C16	119.17 (11)	C14—C15—H15	120.00
C11—C16—C15	120.98 (12)	C16—C15—H15	120.00
C1—C21—C22	119.31 (10)	C11—C16—H16	120.00
C1—C21—C26	122.37 (11)	C15—C16—H16	119.00

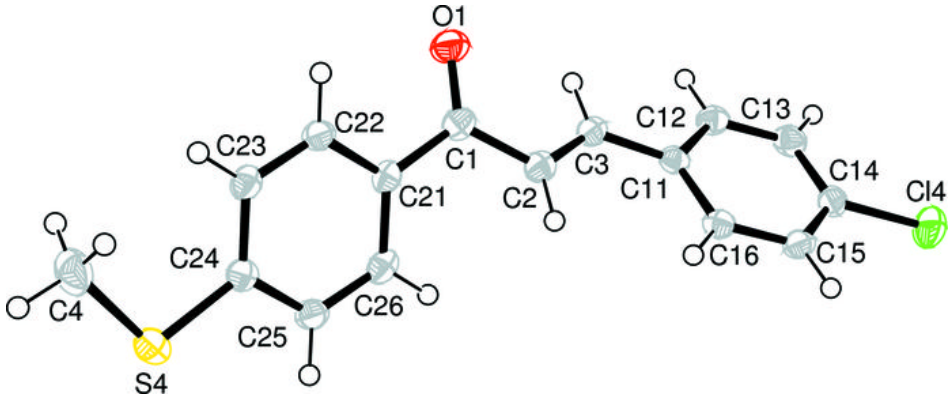
C22—C21—C26	118.31 (12)	C21—C22—H22	119.00
C21—C22—C23	121.62 (11)	C23—C22—H22	119.00
C22—C23—C24	119.59 (11)	C22—C23—H23	120.00
S4—C24—C23	124.46 (10)	C24—C23—H23	120.00
S4—C24—C25	116.56 (9)	C24—C25—H25	120.00
C23—C24—C25	118.98 (12)	C26—C25—H25	120.00
C24—C25—C26	120.98 (11)	C21—C26—H26	120.00
C21—C26—C25	120.47 (12)	C25—C26—H26	120.00
C4—S4—C24—C23	2.51 (12)	C12—C13—C14—C15	−0.84 (19)
C4—S4—C24—C25	−177.35 (10)	C12—C13—C14—Cl4	179.71 (10)
O1—C1—C2—C3	21.2 (2)	Cl4—C14—C15—C16	179.25 (10)
O1—C1—C21—C26	−159.89 (12)	C13—C14—C15—C16	−0.20 (19)
C21—C1—C2—C3	−159.94 (12)	C14—C15—C16—C11	1.15 (18)
O1—C1—C21—C22	19.52 (18)	C1—C21—C26—C25	177.59 (12)
C2—C1—C21—C26	21.23 (18)	C22—C21—C26—C25	−1.83 (18)
C2—C1—C21—C22	−159.36 (11)	C1—C21—C22—C23	−179.31 (11)
C1—C2—C3—C11	−173.63 (12)	C26—C21—C22—C23	0.13 (18)
C2—C3—C11—C12	−173.92 (13)	C21—C22—C23—C24	1.01 (17)
C2—C3—C11—C16	10.4 (2)	C22—C23—C24—C25	−0.47 (17)
C16—C11—C12—C13	−0.07 (18)	C22—C23—C24—S4	179.67 (9)
C3—C11—C12—C13	−175.92 (12)	S4—C24—C25—C26	178.65 (10)
C12—C11—C16—C15	−1.01 (17)	C23—C24—C25—C26	−1.23 (18)
C3—C11—C16—C15	174.71 (12)	C24—C25—C26—C21	2.40 (19)
C11—C12—C13—C14	0.98 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···Cg^{i}	0.95	2.81	3.527 (1)	133
C22—H22···Cg^{ii}	0.95	2.94	3.550 (1)	124

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) *x*, −*y*+1/2, *z*+1/2.

Fig. 1


O1
C22
C23
C1
C21
C2
C3
C12
C13
C14
Cl4
C11
C16
C15
C24
C4
C26
C25
S4