

# 3-(4-Chlorophenyl)-3-hydroxy-1-phenylprop-2-ene-1-thione

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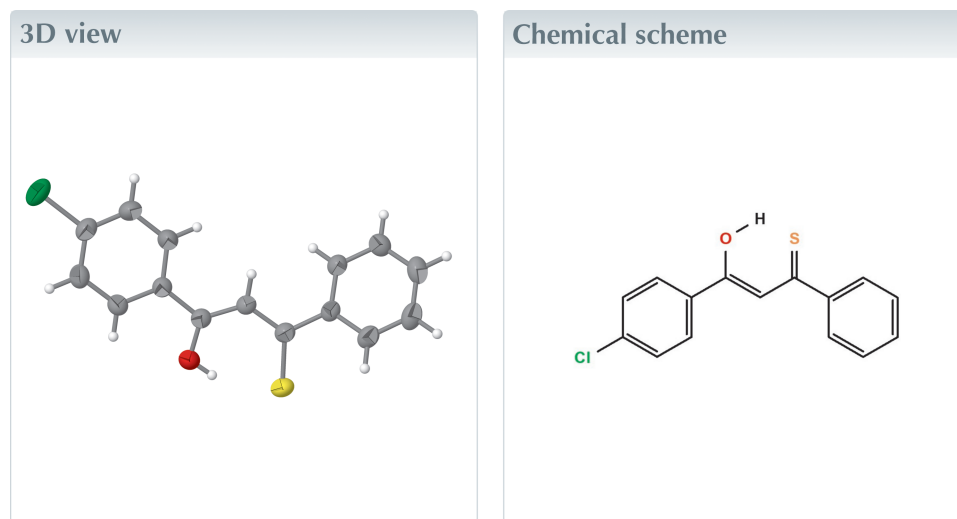
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**Keywords:** chlorophenyl; thioxopropan; dihedral angle; crystal structure.

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**Structural data:** full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the title compound, C<sub>15</sub>H<sub>11</sub>ClOS, the dihedral angle between the aromatic rings is 13.06 (6)° and an intramolecular O—H···S hydrogen bond supports the molecular conformation. In the extended structure, weak C—H···O hydrogen bonds connect the molecules into [010] chains.



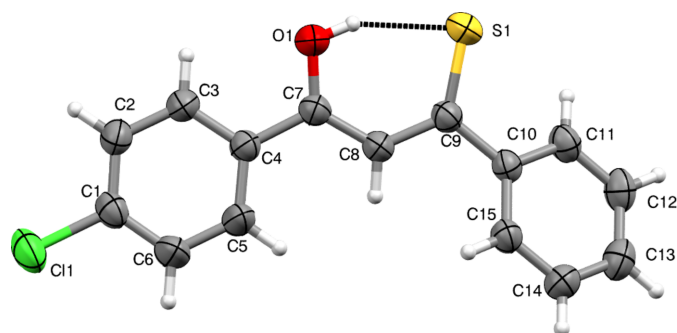
## Structure description

The title compound, C<sub>15</sub>H<sub>11</sub>ClOS, adopts a non-planar structure (Fig. 1) defined by the dihedral angle between the mean planes of the C1–C6 and C10–C16 phenyl rings of 13.06 (6)°. The major twist in the molecule occurs about the C9–C10 bond [C8–C9–C10–C15 = –32.1 (2)°] and an intramolecular O—H···S hydrogen bond (Table 1) supports the conformation. The bond lengths and bond angles are in good agreement with literature values for similar structures (Ganesha *et al.* 2023; Sreenatha *et al.* 2018, 2021; Nizamuddin *et al.* 2025; Lakshminarayana *et al.* 2022).

In the extended structure, weak C—H···O hydrogen bonds connect the molecules into C(6) [010] chains (Fig. 2) with adjacent molecules related by glide symmetry.

## Synthesis and crystallization

To a stirred suspension of NaH (0.175 g, 2 eq.) in 20 ml of *N,N*-dimethylformamide (DMF) was added 4-chloroacetophenone (1.00 g, 1 eq.) dropwise and the suspension was stirred at room temperature (Fig. 3). After 1 h, phenyldithioester (0.672 g, 1.1 eq.) dissolved in 20 ml of DMF was added dropwise and the stirring was continued at room temperature. After completion of the reaction (monitored by TLC), it was quenched with saturated aqueous NH<sub>4</sub>OH solution (50 ml) extracted with EtOAc (3 × 25 ml), washed with water (3 × 25 ml), brine (25 ml), and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The combined



**Figure 1**  
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

organic layer was evaporated under vacuum to give the title compound (single spot on TLC), which was passed through a silica gel column for further purification using hexane/EtOAc (9.5:0.5), as eluent. Then, 0.5 g of the title compound was dissolved in 10 ml of DMF and was allowed to undergo slow evaporation (Nagaraju *et al.* 2020). Good quality crystals obtained were isolated and subjected to single-crystal X-ray diffraction studies.

### Refinement

Crystal data and structure refinement details are summarized in Table 2.

**Table 1**  
Hydrogen-bond geometry (Å, °).

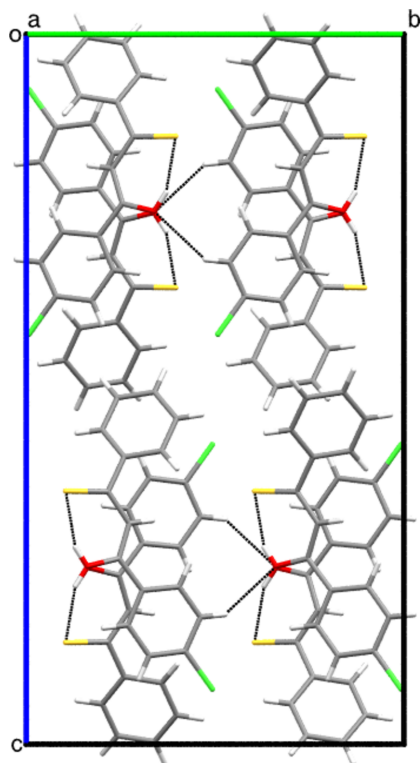
<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O1–H1···S1	0.82	2.11	2.8763 (12)	155
C6–H6···O1 <sup>i</sup>	0.93	2.59	3.379 (2)	143

Symmetry code: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, z$ .

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>15</sub> H <sub>11</sub> ClOS
<i>M<sub>r</sub></i>	274.75
Crystal system, space group	Orthorhombic, <i>Pbca</i>
Temperature (K)	302
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.2296 (2), 13.8519 (3), 26.0849 (7)
<i>V</i> (Å <sup>3</sup> )	2612.24 (12)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
$\mu$ (mm <sup>-1</sup> )	0.44
Crystal size (mm)	0.28 × 0.25 × 0.23
Data collection	
Diffractometer	Bruker SMART CCD
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	90193, 3984, 3197
<i>R</i> <sub>int</sub>	0.046
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.715
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.042, 0.136, 1.04
No. of reflections	3984
No. of parameters	163
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.27, -0.38

Computer programs: *APEX* and *SAINT* (Bruker, 2012), *SHELXT2014/4* (Sheldrick, 2015a), *SHELXL2019/2* (Sheldrick, 2015b) and *PLATON*(Spek, 2020).



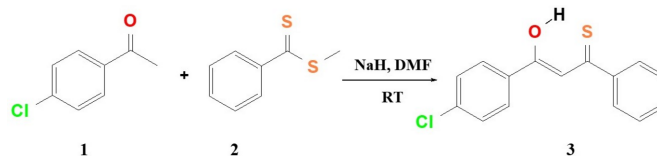
**Figure 2**  
Packing of the title compound viewed along [100] with hydrogen bonds indicated by black dashed lines.

### Acknowledgements

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**Figure 3**  
Synthesis scheme for the title compound.

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## full crystallographic data

*IUCrData* (2026). **11**, x260563 [<https://doi.org/10.1107/S2414314626005638>]

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*Crystal data*

$C_{15}H_{11}ClOS$	$D_x = 1.397 \text{ Mg m}^{-3}$
$M_r = 274.75$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Orthorhombic, <i>Pbca</i>	Cell parameters from 90193 reflections
$a = 7.2296 (2) \text{ \AA}$	$\theta = 3.0\text{--}30.5^\circ$
$b = 13.8519 (3) \text{ \AA}$	$\mu = 0.44 \text{ mm}^{-1}$
$c = 26.0849 (7) \text{ \AA}$	$T = 302 \text{ K}$
$V = 2612.24 (12) \text{ \AA}^3$	Block, colorless
$Z = 8$	$0.28 \times 0.25 \times 0.23 \text{ mm}$
$F(000) = 1136$	

*Data collection*

Bruker SMART CCD diffractometer	3197 reflections with $I > 2\sigma(I)$
Radiation source: graphite	$R_{\text{int}} = 0.046$
$\omega$ scans	$\theta_{\text{max}} = 30.5^\circ$ , $\theta_{\text{min}} = 3.0^\circ$
90193 measured reflections	$h = -10 \rightarrow 10$
3984 independent reflections	$k = -19 \rightarrow 19$
	$l = -36 \rightarrow 36$

*Refinement*

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0742P)^2 + 0.5775P]$
$wR(F^2) = 0.136$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{\text{max}} = 0.001$
3984 reflections	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
163 parameters	$\Delta\rho_{\text{min}} = -0.38 \text{ e \AA}^{-3}$
0 restraints	
Primary atom site location: dual	

*Special details*

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

**Refinement.** Hydrogen atoms were placed in ideal positions and refined as riding model of C—H = 0.93  $\text{\AA}$  with  $U_{\text{iso}}$  (H) = 1.2 $U_{\text{eq}}$  (C) for aromatic H atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.13146 (8)	0.10428 (3)	0.64334 (2)	0.05992 (16)
Cl1	0.32731 (8)	0.49282 (4)	0.92234 (2)	0.06749 (17)
O1	0.12163 (18)	0.16132 (8)	0.74933 (4)	0.0540 (3)
H1	0.108232	0.129925	0.722935	0.081*
C4	0.2303 (2)	0.30758 (10)	0.78307 (5)	0.0388 (3)
C10	0.28603 (18)	0.25950 (10)	0.59518 (5)	0.0376 (3)
C8	0.2416 (2)	0.27248 (10)	0.68877 (5)	0.0395 (3)
H8	0.290559	0.334080	0.684611	0.047*
C3	0.2164 (2)	0.26910 (11)	0.83215 (5)	0.0447 (3)
H3	0.186004	0.204298	0.836171	0.054*
C15	0.2767 (2)	0.35871 (11)	0.58661 (5)	0.0432 (3)
H15	0.227176	0.398827	0.611690	0.052*
C9	0.2216 (2)	0.21652 (10)	0.64414 (5)	0.0393 (3)
C2	0.2469 (2)	0.32550 (12)	0.87512 (6)	0.0486 (3)
H2	0.237457	0.299027	0.907778	0.058*
C7	0.19601 (19)	0.24538 (10)	0.73824 (5)	0.0396 (3)
C11	0.3609 (2)	0.20103 (12)	0.55686 (6)	0.0455 (3)
H11	0.366388	0.134537	0.561551	0.055*
C14	0.3403 (2)	0.39815 (12)	0.54114 (6)	0.0514 (4)
H14	0.331563	0.464328	0.535660	0.062*
C1	0.2911 (2)	0.42091 (12)	0.86880 (6)	0.0464 (3)
C5	0.2752 (3)	0.40477 (11)	0.77817 (6)	0.0576 (4)
H5	0.284178	0.432015	0.745679	0.069*
C12	0.4271 (2)	0.24143 (13)	0.51187 (6)	0.0521 (4)
H12	0.478848	0.201929	0.486868	0.063*
C13	0.4169 (2)	0.33946 (14)	0.50382 (6)	0.0543 (4)
H13	0.461181	0.366107	0.473488	0.065*
C6	0.3067 (3)	0.46137 (12)	0.82081 (7)	0.0624 (5)
H6	0.338160	0.526109	0.817167	0.075*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0890 (3)	0.0388 (2)	0.0519 (3)	-0.01420 (19)	0.0021 (2)	-0.00697 (16)
Cl1	0.0811 (3)	0.0675 (3)	0.0538 (3)	-0.0044 (2)	0.0007 (2)	-0.0245 (2)
O1	0.0793 (8)	0.0396 (5)	0.0432 (5)	-0.0116 (5)	0.0043 (5)	0.0008 (4)
C4	0.0436 (7)	0.0361 (6)	0.0367 (6)	0.0021 (5)	0.0032 (5)	-0.0007 (5)
C10	0.0393 (6)	0.0396 (7)	0.0340 (6)	0.0018 (5)	-0.0037 (5)	-0.0045 (5)
C8	0.0467 (7)	0.0349 (6)	0.0370 (6)	-0.0030 (5)	0.0006 (5)	-0.0018 (5)
C3	0.0541 (8)	0.0412 (7)	0.0388 (7)	-0.0064 (6)	0.0012 (6)	0.0024 (6)
C15	0.0520 (7)	0.0408 (7)	0.0369 (7)	0.0019 (6)	-0.0002 (6)	-0.0036 (5)
C9	0.0430 (7)	0.0361 (6)	0.0387 (7)	0.0015 (5)	-0.0025 (5)	-0.0022 (5)
C2	0.0561 (8)	0.0537 (8)	0.0362 (7)	-0.0054 (7)	0.0015 (6)	0.0004 (6)
C7	0.0445 (7)	0.0356 (6)	0.0387 (7)	0.0012 (5)	0.0004 (5)	-0.0006 (5)
C11	0.0486 (7)	0.0447 (7)	0.0432 (7)	0.0080 (6)	-0.0015 (6)	-0.0083 (6)

C14	0.0619 (9)	0.0472 (8)	0.0450 (8)	-0.0011 (7)	-0.0003 (7)	0.0054 (6)
C1	0.0498 (8)	0.0467 (8)	0.0427 (7)	0.0011 (6)	0.0032 (6)	-0.0104 (6)
C5	0.0960 (13)	0.0371 (7)	0.0396 (7)	-0.0016 (8)	0.0063 (8)	0.0023 (6)
C12	0.0502 (8)	0.0660 (10)	0.0401 (7)	0.0089 (7)	0.0032 (6)	-0.0100 (7)
C13	0.0554 (9)	0.0685 (11)	0.0390 (7)	-0.0003 (8)	0.0043 (6)	0.0041 (7)
C6	0.1009 (14)	0.0359 (7)	0.0503 (9)	-0.0051 (8)	0.0081 (9)	-0.0048 (7)

*Geometric parameters (Å, °)*

S1—C9	1.6860 (15)	C15—C14	1.384 (2)
C11—C1	1.7353 (15)	C15—H15	0.9300
O1—C7	1.3148 (17)	C2—C1	1.370 (2)
O1—H1	0.8200	C2—H2	0.9300
C4—C5	1.391 (2)	C11—C12	1.385 (2)
C4—C3	1.3904 (19)	C11—H11	0.9300
C4—C7	1.4736 (18)	C14—C13	1.384 (2)
C10—C15	1.3940 (19)	C14—H14	0.9300
C10—C11	1.3959 (19)	C1—C6	1.376 (2)
C10—C9	1.4841 (19)	C5—C6	1.380 (2)
C8—C7	1.3837 (19)	C5—H5	0.9300
C8—C9	1.4060 (18)	C12—C13	1.376 (3)
C8—H8	0.9300	C12—H12	0.9300
C3—C2	1.384 (2)	C13—H13	0.9300
C3—H3	0.9300	C6—H6	0.9300
C7—O1—H1	109.5	O1—C7—C4	114.33 (12)
C5—C4—C3	118.21 (13)	C8—C7—C4	122.77 (12)
C5—C4—C7	122.16 (13)	C12—C11—C10	120.41 (15)
C3—C4—C7	119.63 (12)	C12—C11—H11	119.8
C15—C10—C11	118.42 (14)	C10—C11—H11	119.8
C15—C10—C9	121.22 (12)	C13—C14—C15	120.25 (16)
C11—C10—C9	120.34 (13)	C13—C14—H14	119.9
C7—C8—C9	126.72 (13)	C15—C14—H14	119.9
C7—C8—H8	116.6	C2—C1—C6	121.43 (14)
C9—C8—H8	116.6	C2—C1—C11	119.48 (12)
C2—C3—C4	121.18 (14)	C6—C1—C11	119.08 (13)
C2—C3—H3	119.4	C6—C5—C4	120.96 (15)
C4—C3—H3	119.4	C6—C5—H5	119.5
C14—C15—C10	120.68 (14)	C4—C5—H5	119.5
C14—C15—H15	119.7	C13—C12—C11	120.63 (14)
C10—C15—H15	119.7	C13—C12—H12	119.7
C8—C9—C10	117.33 (12)	C11—C12—H12	119.7
C8—C9—S1	123.95 (11)	C12—C13—C14	119.59 (15)
C10—C9—S1	118.72 (10)	C12—C13—H13	120.2
C1—C2—C3	118.97 (14)	C14—C13—H13	120.2
C1—C2—H2	120.5	C1—C6—C5	119.24 (15)
C3—C2—H2	120.5	C1—C6—H6	120.4
O1—C7—C8	122.88 (13)	C5—C6—H6	120.4

C5—C4—C3—C2	-0.2 (2)	C5—C4—C7—C8	13.5 (2)
C7—C4—C3—C2	-179.73 (15)	C3—C4—C7—C8	-167.04 (14)
C11—C10—C15—C14	0.0 (2)	C15—C10—C11—C12	1.1 (2)
C9—C10—C15—C14	178.81 (14)	C9—C10—C11—C12	-177.71 (14)
C7—C8—C9—C10	-177.99 (13)	C10—C15—C14—C13	-1.0 (2)
C7—C8—C9—S1	1.4 (2)	C3—C2—C1—C6	-0.4 (3)
C15—C10—C9—C8	-32.1 (2)	C3—C2—C1—C11	179.30 (13)
C11—C10—C9—C8	146.74 (14)	C3—C4—C5—C6	0.5 (3)
C15—C10—C9—S1	148.47 (12)	C7—C4—C5—C6	-179.97 (17)
C11—C10—C9—S1	-32.71 (18)	C10—C11—C12—C13	-1.2 (2)
C4—C3—C2—C1	0.1 (2)	C11—C12—C13—C14	0.2 (3)
C9—C8—C7—O1	-1.7 (2)	C15—C14—C13—C12	0.9 (3)
C9—C8—C7—C4	177.02 (14)	C2—C1—C6—C5	0.7 (3)
C5—C4—C7—O1	-167.72 (15)	C11—C1—C6—C5	-178.99 (16)
C3—C4—C7—O1	11.8 (2)	C4—C5—C6—C1	-0.8 (3)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1—H1 $\cdots$ S1	0.82	2.11	2.8763 (12)	155
C6—H6 $\cdots$ O1 <sup>i</sup>	0.93	2.59	3.379 (2)	143

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