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ISSN 2414-3146

5-(4-Chlorophenyl)-3-(4-methoxyphenyl)isothiazole

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Received 13 October 2026
Accepted 22 October 2026

Edited by W. T. A. Harrison, University of Aberdeen, United Kingdom

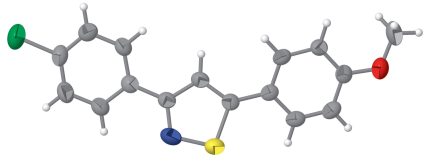
Keywords: chlorophenyl; methoxyphenyl; isothiazole; C—H···N/S interactions; crystal structure.

CCDC reference: 2158969

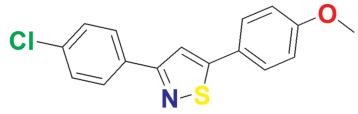
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{16}H_{12}ClNOS$, the dihedral angles between the central isothiazole ring and pendant *p*-methoxyphenyl and *p*-chlorophenyl rings are 19.30 (19) and 13.8 (2)°, respectively. The molecule exhibits short intramolecular C—H···S and C—H···N contacts, each generating an *S*(5) ring motif.

3D view



Chemical scheme



Structure description

The title compound, $C_{16}H_{12}ClNOS$ (**2**), crystallizes with one molecule in the asymmetric unit (Fig. 1) in space group *Cc*. The dihedral angles between the central C1/C2/C3/S1/N1 isothiazole ring and pendant C4–C9 *p*-methoxyphenyl and C11–C16 *p*-chlorophenyl rings are 19.30 (19) and 13.8 (2)°, respectively. The dihedral angle between the pendant rings is 15.9 (2)°. The inter-ring bond distances of C1—C11 = 1.472 (6) Å and C3—C4 = 1.461 (5) Å are very similar. Otherwise, all the bond distances in **2** are consistent with those in related structures (Chakravarthy *et al.*, 2026; Sreenatha *et al.*, 2020; Sreenatha *et al.*, 2018). The molecular conformation of **2** is supported by short intramolecular C9—H9···S1 and C12—H12···N1 contacts (Table 1): both of these enclose an *S*(5) ring. The packing of the molecules is shown in Fig. 2.

Synthesis and crystallization

Compound **2** was synthesized by following a literature procedure (Zhang *et al.*, 2021) (Fig. 3). A vessel was charged with **1** (0.20 mmol), Na_2S (0.30 mmol, 23.4 mg), $NaHCO_3$ (0.40 mmol, 33.6 mg) and H_2O (1.20 mmol, 21.6 mg) in *N*,*N*-dimethylformamide (DMF) (2 ml). The reaction mixture was stirred at 90°C in an oil bath for 13–15 h until the starting material was consumed completely as monitored by TLC. After the completion of the reaction the mixture was poured into ethyl acetate and washed with brine (2 × 15 ml). The combined organic layers were dried over anhydrous $MgSO_4$ and evaporated

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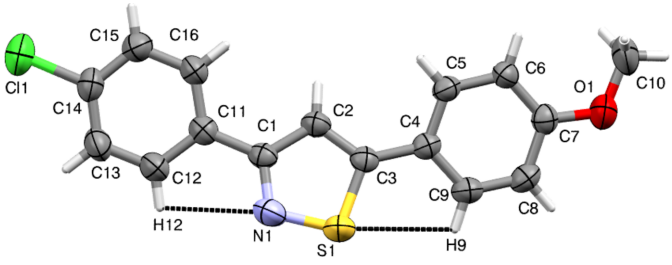


Figure 1
The molecular structure of **2** drawn at 50% probability with short intramolecular contacts represented by dashed lines.

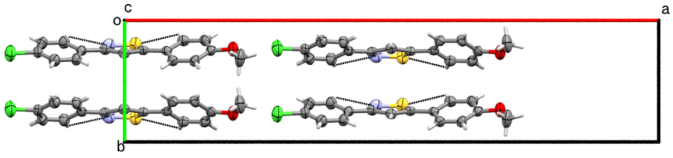


Figure 2
The packing for **2** viewed along the crystallographic *c* axis.

under vacuum. The residue was purified by flash column chromatography using petroleum ether/ethyl acetate as the eluent to afford the desired product **2** in 87% yield. Then, 0.5 g of **2** was dissolved in 5 ml of DMF and was allowed to undergo slow evaporation to form colorless blocks.

Refinement

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

Acknowledgements

The authors are thankful to the BMSIT&M, Bengaluru, and the GEC, Chamarajanagara for support.

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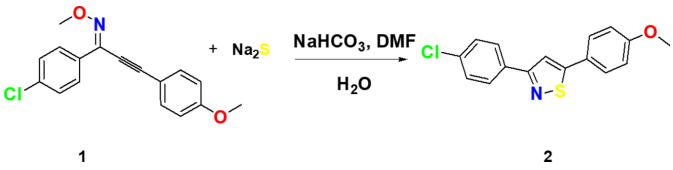


Figure 3
Synthesis scheme for **2**.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···S1	0.93	2.77	3.155 (4)	106
C12—H12···N1	0.93	2.55	2.857 (6)	100

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{12}ClNOS$
M_r	301.78
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	301
a, *b*, *c* (Å)	32.054 (3), 7.2423 (7), 6.0942 (5)
β (°)	93.607 (3)
V (Å^3)	1411.9 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.41
Crystal size (mm)	0.30 × 0.27 × 0.21
Data collection	
Diffractometer	Bruker APEXII
Absorption correction	Multi-scan (Krause *et al.*, 2015)
T_{min}, T_{max}	0.677, 0.739
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	43343, 4353, 2555
R_{int}	0.094
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.121, 1.01
No. of reflections	4353
No. of parameters	182
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.25
Absolute structure	Flack *x* determined using 978 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.05 (3)

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXT2014/4* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *PLATON*(Spek, 2020).

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full crystallographic data

IUCrData (2026). **11**, x261098 [https://doi.org/10.1107/S2414314626010989]

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5-(4-Chlorophenyl)-3-(4-methoxyphenyl)-1,2-thiazole

Crystal data

$C_{16}H_{12}ClNOS$
M_r = 301.78
Monoclinic, *Cc*
a = 32.054 (3) Å
b = 7.2423 (7) Å
c = 6.0942 (5) Å
β = 93.607 (3)°
V = 1411.9 (2) Å^3
Z = 4
F(000) = 624.0
D_x = 1.420 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4353 reflections
θ = 2.6–30.5°
μ = 0.41 mm^{-1}
T = 301 K
Block, colorless
0.30 × 0.27 × 0.21 mm

Data collection

Bruker APEX diffractometer
Radiation source: graphite
SAINT (Bruker, 2012) scans
Absorption correction: multi-scan (Krause *et al.*, 2015)
T_{min} = 0.677, T_{max} = 0.739
43343 measured reflections
4353 independent reflections
2555 reflections with $I > 2\sigma(I)$
R_{int} = 0.094
θ_{max} = 30.5°, θ_{min} = 2.6°
h = −45→45
k = −10→10
l = −8→8
4353 standard reflections every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.121
S = 1.01
4353 reflections
182 parameters
2 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 0.4728P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.018
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack *x* determined using 978 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.05 (3)

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. The methyl H atoms were placed in calculated positions and refined as riding atoms with U_{iso}(H) = 1.5U_{eq}(C). All other H atoms were positioned geometrically and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.47015 (14)	0.7064 (5)	0.7742 (6)	0.0591 (11)
S1	0.52016 (4)	0.70064 (18)	0.83327 (15)	0.0599 (3)
O1	0.70313 (10)	0.7362 (5)	0.3621 (6)	0.0636 (9)
Cl1	0.28598 (4)	0.7711 (2)	0.1759 (2)	0.0833 (5)
C1	0.46277 (13)	0.7425 (5)	0.5613 (7)	0.0400 (9)
C2	0.49908 (13)	0.7689 (5)	0.4444 (6)	0.0418 (9)
C3	0.53505 (13)	0.7466 (5)	0.5741 (6)	0.0395 (8)
C4	0.57864 (12)	0.7502 (5)	0.5173 (6)	0.0382 (8)
C5	0.59000 (12)	0.8323 (6)	0.3257 (6)	0.0434 (9)
C6	0.63132 (12)	0.8324 (6)	0.2661 (7)	0.0446 (9)
C7	0.66182 (13)	0.7482 (6)	0.4015 (7)	0.0433 (9)
C8	0.65076 (13)	0.6660 (6)	0.5985 (7)	0.0488 (10)
C9	0.61006 (13)	0.6673 (6)	0.6540 (6)	0.0463 (10)
C10	0.71611 (17)	0.8111 (10)	0.1694 (10)	0.0847 (18)
C11	0.41961 (14)	0.7482 (5)	0.4638 (7)	0.0423 (9)
C12	0.38673 (14)	0.6809 (6)	0.5819 (7)	0.0523 (11)
C13	0.34575 (14)	0.6873 (6)	0.4948 (8)	0.0586 (12)
C14	0.33749 (13)	0.7612 (7)	0.2906 (8)	0.0504 (11)
C15	0.36868 (13)	0.8283 (7)	0.1691 (7)	0.0547 (11)
C16	0.40983 (13)	0.8195 (6)	0.2572 (7)	0.0492 (10)
H2	0.498508	0.798179	0.295664	0.050*
H5	0.569576	0.889094	0.233849	0.052*
H6	0.638274	0.888710	0.136228	0.054*
H8	0.671192	0.610591	0.691597	0.059*
H9	0.603131	0.612082	0.784607	0.056*
H10A	0.699173	0.763190	0.046890	0.127*
H10B	0.744828	0.779184	0.153505	0.127*
H10C	0.713348	0.943035	0.173878	0.127*
H12	0.392495	0.630994	0.721126	0.063*
H13	0.324164	0.641881	0.574405	0.070*
H15	0.362514	0.878733	0.030485	0.066*
H16	0.431213	0.862731	0.174619	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.065 (3)	0.068 (3)	0.045 (2)	−0.0046 (19)	0.0129 (18)	0.0084 (18)
S1	0.0563 (7)	0.0828 (8)	0.0403 (5)	−0.0031 (7)	0.0017 (4)	0.0113 (6)
O1	0.0416 (15)	0.081 (2)	0.068 (2)	0.0024 (16)	0.0012 (14)	0.0022 (19)
Cl1	0.0460 (7)	0.1072 (12)	0.0954 (11)	−0.0022 (7)	−0.0064 (6)	0.0041 (9)
C1	0.047 (2)	0.035 (2)	0.039 (2)	0.0026 (16)	0.0063 (16)	0.0020 (15)
C2	0.048 (2)	0.043 (2)	0.0353 (19)	0.0012 (17)	0.0060 (16)	−0.0001 (15)

C3	0.045 (2)	0.032 (2)	0.041 (2)	−0.0021 (17)	0.0032 (16)	0.0017 (15)
C4	0.045 (2)	0.031 (2)	0.038 (2)	−0.0013 (15)	−0.0020 (15)	−0.0016 (14)
C5	0.046 (2)	0.044 (2)	0.039 (2)	−0.0006 (17)	−0.0050 (17)	0.0050 (17)
C6	0.042 (2)	0.050 (2)	0.041 (2)	−0.0063 (18)	0.0013 (16)	0.0064 (17)
C7	0.041 (2)	0.042 (2)	0.047 (2)	−0.0055 (18)	0.0005 (16)	−0.0048 (17)
C8	0.051 (3)	0.046 (3)	0.048 (2)	0.0055 (18)	−0.0084 (18)	0.0032 (18)
C9	0.055 (2)	0.045 (2)	0.038 (2)	0.0001 (18)	−0.0005 (17)	0.0036 (16)
C10	0.041 (3)	0.130 (5)	0.084 (4)	−0.012 (3)	0.013 (3)	0.006 (4)
C11	0.046 (2)	0.036 (2)	0.045 (2)	0.0000 (17)	0.0069 (17)	−0.0023 (17)
C12	0.049 (3)	0.060 (3)	0.049 (2)	−0.001 (2)	0.0104 (19)	0.006 (2)
C13	0.043 (2)	0.063 (3)	0.071 (3)	−0.006 (2)	0.012 (2)	0.009 (2)
C14	0.037 (2)	0.049 (3)	0.064 (3)	0.0015 (18)	−0.0004 (19)	−0.003 (2)
C15	0.054 (3)	0.059 (3)	0.050 (3)	−0.001 (2)	−0.002 (2)	0.0057 (19)
C16	0.043 (2)	0.056 (3)	0.049 (2)	−0.0029 (19)	0.0094 (18)	0.0049 (19)

Geometric parameters (Å, º)

S1—N1	1.621 (5)	C9—H9	0.9300
S1—C3	1.711 (4)	C11—C16	1.378 (6)
Cl1—C14	1.754 (4)	C11—C12	1.401 (6)
C4—C5	1.380 (5)	C16—C15	1.394 (6)
C4—C9	1.401 (5)	C16—H16	0.9300
C4—C3	1.461 (5)	C6—H6	0.9300
C1—N1	1.330 (5)	C14—C13	1.365 (7)
C1—C2	1.415 (6)	C14—C15	1.370 (6)
C1—C11	1.472 (6)	C15—H15	0.9300
C7—O1	1.363 (5)	C2—H2	0.9300
C7—C6	1.381 (6)	C12—C13	1.386 (6)
C7—C8	1.405 (6)	C12—H12	0.9300
C8—C9	1.368 (6)	C13—H13	0.9300
C8—H8	0.9300	C10—O1	1.381 (6)
C5—C6	1.395 (5)	C10—H10A	0.9600
C5—H5	0.9300	C10—H10B	0.9600
C3—C2	1.366 (5)	C10—H10C	0.9600
N1—S1—C3	96.9 (2)	C11—C16—H16	119.2
C5—C4—C9	118.0 (4)	C15—C16—H16	119.2
C5—C4—C3	121.0 (3)	C7—C6—C5	119.5 (4)
C9—C4—C3	120.9 (4)	C7—C6—H6	120.3
N1—C1—C2	114.6 (4)	C5—C6—H6	120.3
N1—C1—C11	120.3 (4)	C13—C14—C15	121.7 (4)
C2—C1—C11	125.1 (3)	C13—C14—Cl1	120.2 (4)
C1—N1—S1	109.5 (3)	C15—C14—Cl1	118.1 (4)
O1—C7—C6	125.6 (4)	C14—C15—C16	118.7 (4)
O1—C7—C8	115.1 (4)	C14—C15—H15	120.6
C6—C7—C8	119.4 (4)	C16—C15—H15	120.6
C9—C8—C7	120.3 (4)	C3—C2—C1	112.6 (3)
C9—C8—H8	119.9	C3—C2—H2	123.7

C7—C8—H8	119.9	C1—C2—H2	123.7
C4—C5—C6	121.7 (4)	C13—C12—C11	121.1 (4)
C4—C5—H5	119.1	C13—C12—H12	119.4
C6—C5—H5	119.1	C11—C12—H12	119.4
C2—C3—C4	130.2 (4)	C14—C13—C12	119.1 (4)
C2—C3—S1	106.4 (3)	C14—C13—H13	120.4
C4—C3—S1	123.3 (3)	C12—C13—H13	120.4
C8—C9—C4	121.1 (4)	O1—C10—H10A	109.5
C8—C9—H9	119.4	O1—C10—H10B	109.5
C4—C9—H9	119.4	H10A—C10—H10B	109.5
C16—C11—C12	117.7 (4)	O1—C10—H10C	109.5
C16—C11—C1	122.2 (4)	H10A—C10—H10C	109.5
C12—C11—C1	120.1 (4)	H10B—C10—H10C	109.5
C11—C16—C15	121.6 (4)	C7—O1—C10	118.2 (4)
C2—C1—N1—S1	−0.9 (5)	C12—C11—C16—C15	1.3 (6)
C11—C1—N1—S1	177.7 (3)	C1—C11—C16—C15	−178.4 (4)
C3—S1—N1—C1	0.0 (3)	O1—C7—C6—C5	179.2 (4)
O1—C7—C8—C9	−179.1 (4)	C8—C7—C6—C5	−0.9 (6)
C6—C7—C8—C9	0.9 (6)	C4—C5—C6—C7	0.1 (6)
C9—C4—C5—C6	0.6 (6)	C13—C14—C15—C16	0.3 (7)
C3—C4—C5—C6	−178.2 (4)	Cl1—C14—C15—C16	−179.3 (4)
C5—C4—C3—C2	19.7 (6)	C11—C16—C15—C14	−1.1 (7)
C9—C4—C3—C2	−159.1 (4)	C4—C3—C2—C1	175.8 (4)
C5—C4—C3—S1	−163.3 (3)	S1—C3—C2—C1	−1.6 (4)
C9—C4—C3—S1	17.9 (5)	N1—C1—C2—C3	1.7 (5)
N1—S1—C3—C2	1.0 (3)	C11—C1—C2—C3	−176.8 (4)
N1—S1—C3—C4	−176.6 (3)	C16—C11—C12—C13	−0.6 (6)
C7—C8—C9—C4	−0.2 (6)	C1—C11—C12—C13	179.0 (4)
C5—C4—C9—C8	−0.6 (6)	C15—C14—C13—C12	0.3 (8)
C3—C4—C9—C8	178.3 (4)	Cl1—C14—C13—C12	179.9 (4)
N1—C1—C11—C16	167.0 (4)	C11—C12—C13—C14	−0.2 (7)
C2—C1—C11—C16	−14.5 (6)	C6—C7—O1—C10	−1.2 (6)
N1—C1—C11—C12	−12.6 (6)	C8—C7—O1—C10	178.9 (5)
C2—C1—C11—C12	165.9 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···S1	0.93	2.77	3.155 (4)	106
C12—H12···N1	0.93	2.55	2.857 (6)	100