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2-[4-(4-Methoxyphenyl)-1,3-thiazol-2-yl]-2,3-dihydro-1*H*-isoindole-1,3-dione

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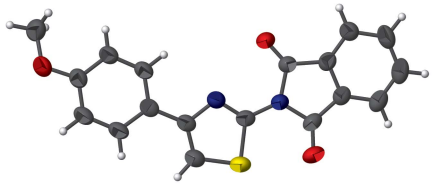
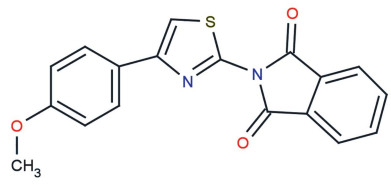
Structural data: full structural data are available from iucrdata.iucr.org

In the title isoindole, $C_{18}H_{12}N_2O_3S$, the methoxyphenyl ring is oriented at an angle of 9.5 (1)° with respect to the thiazole ring. In the crystal, molecules are linked *via* C—H···O interactions, which form $C(7)$ chains propagating along [010]. In addition to this, weak π–π interactions are also observed.

3D view



Chemical scheme



Structure description

In a continuation of our work on the crystal structure analysis of isoindole derivatives, we have undertaken a single-crystal X-ray diffraction study for the title compound, and the results are presented here.

The molecular structure of the title compound is illustrated in Fig. 1. The thiazole ring is planar with a maximum deviation of −0.003 (3) Å for atom C7. The keto O atoms O2 and O3 deviate from the mean plane of the ring to which they are attached by −0.030 (3) and 0.090 (3) Å, respectively. The methoxy group atoms (O1 and C18) deviate by −0.009 (3) and 0.314 (4) Å, respectively, from the best plane of the methoxyphenyl ring. This ring makes a dihedral angle of 9.5 (1)° with thiazole ring. The methoxy phenyl ring is oriented at an angle of 5.2 (1)° with respect to the isoindole ring system. The molecular structure is influenced by an intramolecular C—H···N hydrogen bond (Table 1).

In the crystal, C—H···O interactions link the molecules, forming $C(7)$ chains propagating along along the *b* axis, see Fig. 2. In addition, π–π interactions are also observed between the centroids of the benzene rings (C1–C6) and (C11–C16) at $(-1 + x, \frac{1}{2} - y, -\frac{1}{2} + z)$ with a centroid–centroid distance of 3.740 (5) Å, see Fig. 3.

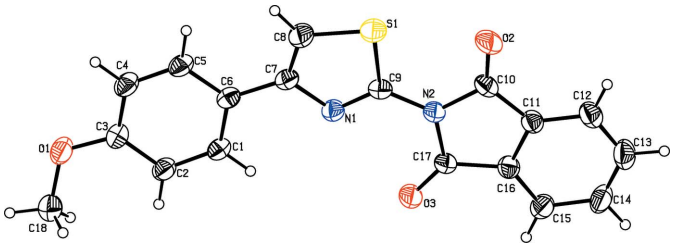


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

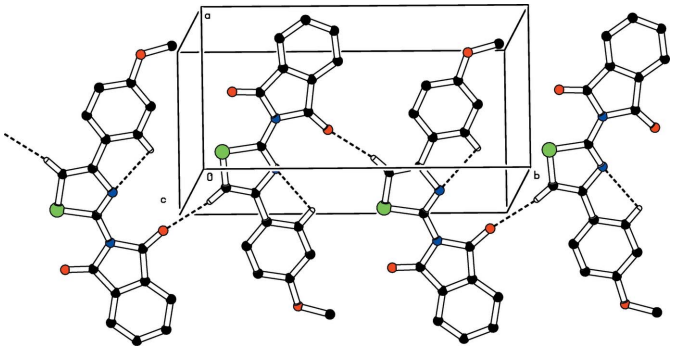


Figure 2
Crystal packing of the title compound, viewed along the *c* axis. The C—H···N and C—H···O hydrogen bonds are shown as dashed lines (see Table 1). For clarity, H atoms not involved in these hydrogen bonds have been omitted.

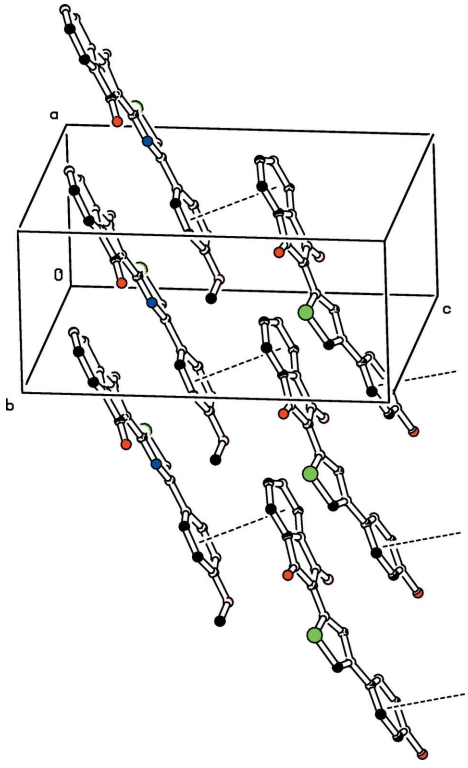


Figure 3
The packing of the title compound, showing π–π interactions as dashed lines. For clarity, H atoms have been omitted.

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···N1	0.93	2.52	2.853 (5)	102
C8—H8···O3^{i}	0.93	2.36	3.282 (5)	171

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{12}N_2O_3S$
M_r	336.36
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	7.004 (9), 14.054 (17), 15.275 (19)
β (°)	90.368 (12)
V (Å^3)	1504 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.24
Crystal size (mm)	0.22 × 0.20 × 0.18
Data collection	
Diffractometer	Bruker SMART APEX CCD area-detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4938, 3280, 2012
R_{int}	0.057
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.066, 0.219, 1.07
No. of reflections	3280
No. of parameters	217
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.38

Computer programs: *SMART* and *SAINT* (Bruker, 2002), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Synthesis and crystallization

A mixture of 4-(4-methoxyphenyl) thiazol-2-amine (300 mg, 1.46 mmol), phthalic anhydride (431 mmol, 2.92 mmol) in glacial acetic acid (5 ml) was refluxed for 3 h. After cooling, the resulting solid was collected by filtration, washed with petroleum–ether and dried under vacuum giving a yellow solid. The solid was further recrystallized from DMF to yield yellow crystals of the title compound.

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161053 [https://doi.org/10.1107/S2414314616010531]

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2-[4-(4-Methoxyphenyl)-1,3-thiazol-2-yl]-2,3-dihydro-1*H*-isoindole-1,3-dione

Crystal data

$C_{18}H_{12}N_2O_3S$
M_r = 336.36
Monoclinic, $P2_1/c$
a = 7.004 (9) Å
b = 14.054 (17) Å
c = 15.275 (19) Å
β = 90.368 (12)°
V = 1504 (3) Å^3
Z = 4
$F(000)$ = 696
D_x = 1.486 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3920 reflections
θ = 3.2–27.2°
μ = 0.24 mm^{-1}
T = 296 K
Block, yellow
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω scans
4938 measured reflections
3280 independent reflections
2012 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −8→8
k = −18→11
l = −19→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.219
S = 1.07
3280 reflections
217 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1064P)^2 + 0.3164P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-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.

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.16107 (14)	0.07298 (6)	0.19904 (7)	0.0674 (4)
O1	−0.7223 (3)	0.31712 (18)	0.44991 (16)	0.0653 (7)

O2	0.5105 (4)	0.10061 (17)	0.12684 (18)	0.0691 (7)
O3	0.2926 (3)	0.39658 (16)	0.19483 (18)	0.0650 (7)
N1	0.0707 (3)	0.23879 (18)	0.25350 (16)	0.0470 (6)
N2	0.3584 (3)	0.23623 (17)	0.17360 (16)	0.0462 (6)
C1	−0.2631 (4)	0.3122 (2)	0.3356 (2)	0.0508 (7)
H1	−0.1709	0.3534	0.3139	0.061*
C2	−0.4239 (5)	0.3500 (2)	0.3752 (2)	0.0533 (8)
H2	−0.4399	0.4155	0.3793	0.064*
C3	−0.5604 (4)	0.2885 (2)	0.40857 (19)	0.0511 (7)
C4	−0.5327 (5)	0.1922 (2)	0.4020 (2)	0.0572 (8)
H4	−0.6231	0.1509	0.4252	0.069*
C5	−0.3740 (5)	0.1556 (2)	0.3620 (2)	0.0541 (8)
H5	−0.3588	0.0901	0.3579	0.065*
C6	−0.2357 (4)	0.2155 (2)	0.32758 (18)	0.0466 (7)
C7	−0.0704 (4)	0.1775 (2)	0.2808 (2)	0.0476 (7)
C8	−0.0427 (5)	0.0870 (2)	0.2574 (2)	0.0644 (9)
H8	−0.1252	0.0375	0.2715	0.077*
C9	0.1984 (4)	0.1926 (2)	0.21012 (19)	0.0465 (7)
C10	0.5085 (4)	0.1856 (2)	0.1338 (2)	0.0517 (8)
C11	0.6487 (4)	0.2556 (2)	0.10617 (19)	0.0493 (7)
C12	0.8216 (5)	0.2432 (3)	0.0653 (2)	0.0599 (9)
H12	0.8638	0.1831	0.0489	0.072*
C13	0.9286 (5)	0.3222 (3)	0.0497 (2)	0.0702 (10)
H13	1.0455	0.3159	0.0218	0.084*
C14	0.8681 (5)	0.4103 (3)	0.0741 (2)	0.0703 (10)
H14	0.9460	0.4627	0.0640	0.084*
C15	0.6925 (5)	0.4233 (2)	0.1137 (2)	0.0609 (9)
H15	0.6499	0.4835	0.1295	0.073*
C16	0.5847 (4)	0.3441 (2)	0.12852 (19)	0.0485 (7)
C17	0.3955 (4)	0.3349 (2)	0.17011 (19)	0.0460 (7)
C18	−0.7772 (6)	0.4126 (3)	0.4398 (3)	0.0757 (11)
H18A	−0.8925	0.4239	0.4718	0.114*
H18B	−0.6778	0.4533	0.4619	0.114*
H18C	−0.7988	0.4259	0.3789	0.114*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0750 (7)	0.0361 (4)	0.0914 (7)	−0.0012 (4)	0.0164 (5)	−0.0021 (4)
O1	0.0654 (15)	0.0593 (15)	0.0715 (15)	−0.0119 (12)	0.0227 (12)	−0.0007 (12)
O2	0.0732 (16)	0.0427 (13)	0.0914 (18)	0.0122 (12)	0.0095 (13)	−0.0082 (12)
O3	0.0631 (14)	0.0388 (12)	0.0934 (18)	0.0035 (11)	0.0236 (12)	−0.0036 (11)
N1	0.0492 (14)	0.0418 (13)	0.0501 (14)	−0.0023 (11)	0.0015 (11)	0.0001 (10)
N2	0.0479 (13)	0.0359 (12)	0.0548 (14)	0.0022 (11)	0.0045 (11)	−0.0008 (10)
C1	0.0549 (18)	0.0438 (16)	0.0536 (17)	−0.0089 (14)	0.0042 (13)	0.0063 (13)
C2	0.0595 (19)	0.0457 (17)	0.0548 (18)	−0.0067 (15)	0.0075 (14)	0.0040 (14)
C3	0.0517 (17)	0.0545 (18)	0.0472 (16)	−0.0084 (15)	0.0053 (13)	−0.0005 (13)
C4	0.063 (2)	0.0468 (17)	0.062 (2)	−0.0150 (16)	0.0085 (15)	0.0017 (14)

C5	0.064 (2)	0.0407 (16)	0.0581 (18)	−0.0119 (15)	0.0051 (15)	0.0040 (14)
C6	0.0521 (16)	0.0464 (16)	0.0412 (15)	−0.0051 (14)	−0.0025 (12)	0.0066 (12)
C7	0.0518 (17)	0.0409 (16)	0.0500 (16)	−0.0050 (13)	−0.0012 (13)	0.0058 (12)
C8	0.065 (2)	0.0449 (18)	0.084 (2)	−0.0075 (16)	0.0127 (18)	0.0017 (16)
C9	0.0518 (16)	0.0380 (14)	0.0496 (16)	0.0016 (13)	−0.0037 (13)	0.0023 (12)
C10	0.0529 (18)	0.0464 (17)	0.0559 (18)	0.0133 (14)	0.0012 (14)	−0.0046 (13)
C11	0.0490 (16)	0.0527 (18)	0.0462 (15)	0.0068 (14)	0.0028 (13)	−0.0004 (13)
C12	0.0555 (19)	0.069 (2)	0.0551 (19)	0.0144 (17)	0.0050 (15)	−0.0047 (16)
C13	0.056 (2)	0.097 (3)	0.058 (2)	0.008 (2)	0.0157 (16)	0.002 (2)
C14	0.059 (2)	0.080 (3)	0.072 (2)	−0.0131 (19)	0.0181 (17)	0.012 (2)
C15	0.065 (2)	0.0519 (19)	0.066 (2)	−0.0031 (17)	0.0146 (16)	0.0019 (16)
C16	0.0520 (17)	0.0507 (17)	0.0428 (15)	0.0059 (14)	0.0058 (12)	−0.0005 (13)
C17	0.0472 (16)	0.0390 (15)	0.0516 (16)	0.0032 (13)	0.0014 (12)	0.0008 (12)
C18	0.073 (2)	0.068 (3)	0.086 (3)	0.007 (2)	0.027 (2)	0.008 (2)

Geometric parameters (Å, º)

S1—C8	1.699 (4)	C5—H5	0.9300
S1—C9	1.710 (4)	C6—C7	1.466 (4)
O1—C3	1.362 (4)	C7—C8	1.335 (5)
O1—C18	1.404 (5)	C8—H8	0.9300
O2—C10	1.199 (4)	C10—C11	1.454 (5)
O3—C17	1.191 (4)	C11—C16	1.366 (4)
N1—C9	1.291 (4)	C11—C12	1.378 (4)
N1—C7	1.378 (4)	C12—C13	1.361 (6)
N2—C9	1.397 (4)	C12—H12	0.9300
N2—C10	1.411 (4)	C13—C14	1.361 (6)
N2—C17	1.411 (4)	C13—H13	0.9300
C1—C6	1.377 (5)	C14—C15	1.386 (5)
C1—C2	1.387 (4)	C14—H14	0.9300
C1—H1	0.9300	C15—C16	1.365 (5)
C2—C3	1.387 (4)	C15—H15	0.9300
C2—H2	0.9300	C16—C17	1.479 (4)
C3—C4	1.372 (5)	C18—H18A	0.9600
C4—C5	1.372 (5)	C18—H18B	0.9600
C4—H4	0.9300	C18—H18C	0.9600
C5—C6	1.389 (4)		

C8—S1—C9	87.85 (16)	N2—C9—S1	121.0 (2)
C3—O1—C18	117.3 (3)	O2—C10—N2	123.3 (3)
C9—N1—C7	110.0 (3)	O2—C10—C11	129.8 (3)
C9—N2—C10	123.6 (3)	N2—C10—C11	106.9 (3)
C9—N2—C17	126.5 (2)	C16—C11—C12	121.3 (3)
C10—N2—C17	110.0 (3)	C16—C11—C10	108.7 (3)
C6—C1—C2	122.0 (3)	C12—C11—C10	130.1 (3)
C6—C1—H1	119.0	C13—C12—C11	117.6 (3)
C2—C1—H1	119.0	C13—C12—H12	121.2
C3—C2—C1	119.0 (3)	C11—C12—H12	121.2

C3—C2—H2	120.5	C14—C13—C12	121.4 (3)
C1—C2—H2	120.5	C14—C13—H13	119.3
O1—C3—C4	116.3 (3)	C12—C13—H13	119.3
O1—C3—C2	124.4 (3)	C13—C14—C15	121.2 (4)
C4—C3—C2	119.3 (3)	C13—C14—H14	119.4
C5—C4—C3	121.1 (3)	C15—C14—H14	119.4
C5—C4—H4	119.4	C16—C15—C14	117.3 (3)
C3—C4—H4	119.4	C16—C15—H15	121.3
C4—C5—C6	120.7 (3)	C14—C15—H15	121.3
C4—C5—H5	119.6	C15—C16—C11	121.2 (3)
C6—C5—H5	119.6	C15—C16—C17	129.8 (3)
C1—C6—C5	117.8 (3)	C11—C16—C17	108.9 (3)
C1—C6—C7	121.0 (3)	O3—C17—N2	126.3 (3)
C5—C6—C7	121.2 (3)	O3—C17—C16	128.2 (3)
C8—C7—N1	114.2 (3)	N2—C17—C16	105.5 (2)
C8—C7—C6	126.5 (3)	O1—C18—H18A	109.5
N1—C7—C6	119.3 (3)	O1—C18—H18B	109.5
C7—C8—S1	112.0 (3)	H18A—C18—H18B	109.5
C7—C8—H8	124.0	O1—C18—H18C	109.5
S1—C8—H8	124.0	H18A—C18—H18C	109.5
N1—C9—N2	123.0 (3)	H18B—C18—H18C	109.5
N1—C9—S1	116.0 (2)		

C6—C1—C2—C3	0.7 (5)	C8—S1—C9—N2	−179.8 (3)
C18—O1—C3—C4	−165.4 (3)	C9—N2—C10—O2	1.0 (5)
C18—O1—C3—C2	15.9 (5)	C17—N2—C10—O2	−178.8 (3)
C1—C2—C3—O1	179.0 (3)	C9—N2—C10—C11	−178.6 (2)
C1—C2—C3—C4	0.3 (5)	C17—N2—C10—C11	1.6 (3)
O1—C3—C4—C5	−179.7 (3)	O2—C10—C11—C16	−179.7 (4)
C2—C3—C4—C5	−1.0 (5)	N2—C10—C11—C16	0.0 (3)
C3—C4—C5—C6	0.6 (5)	O2—C10—C11—C12	−0.5 (6)
C2—C1—C6—C5	−1.1 (5)	N2—C10—C11—C12	179.1 (3)
C2—C1—C6—C7	176.2 (3)	C16—C11—C12—C13	1.5 (5)
C4—C5—C6—C1	0.4 (5)	C10—C11—C12—C13	−177.6 (3)
C4—C5—C6—C7	−176.9 (3)	C11—C12—C13—C14	0.5 (5)
C9—N1—C7—C8	0.5 (4)	C12—C13—C14—C15	−1.8 (6)
C9—N1—C7—C6	−176.9 (3)	C13—C14—C15—C16	1.2 (6)
C1—C6—C7—C8	−169.4 (3)	C14—C15—C16—C11	0.8 (5)
C5—C6—C7—C8	7.8 (5)	C14—C15—C16—C17	179.0 (3)
C1—C6—C7—N1	7.7 (4)	C12—C11—C16—C15	−2.1 (5)
C5—C6—C7—N1	−175.1 (3)	C10—C11—C16—C15	177.1 (3)
N1—C7—C8—S1	−0.5 (4)	C12—C11—C16—C17	179.3 (3)
C6—C7—C8—S1	176.7 (2)	C10—C11—C16—C17	−1.4 (4)
C9—S1—C8—C7	0.2 (3)	C9—N2—C17—O3	−3.0 (5)
C7—N1—C9—N2	179.5 (3)	C10—N2—C17—O3	176.7 (3)
C7—N1—C9—S1	−0.3 (3)	C9—N2—C17—C16	177.9 (3)
C10—N2—C9—N1	173.4 (3)	C10—N2—C17—C16	−2.4 (3)
C17—N2—C9—N1	−6.9 (5)	C15—C16—C17—O3	4.9 (6)

C10—N2—C9—S1	−6.8 (4)	C11—C16—C17—O3	−176.7 (3)
C17—N2—C9—S1	172.9 (2)	C15—C16—C17—N2	−176.0 (3)
C8—S1—C9—N1	0.1 (3)	C11—C16—C17—N2	2.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N1	0.93	2.52	2.853 (5)	102
C8—H8···O3^{i}	0.93	2.36	3.282 (5)	171

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