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(E)-2-[4-*tert*-Butyl-5-(2-chlorobenzyl)-thiazol-2-yliminomethyl]phenol

Gao Cao,[a] Ying-Qi Mang[a] and Ai-Xi Hu[b]*

[a]The School of Chemical and Energy Engineering, South China University of Technology, Guangzhou 510640, People's Republic of China, and [b]College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, People's Republic of China
Correspondence e-mail: axhu0731@yahoo.com.cn

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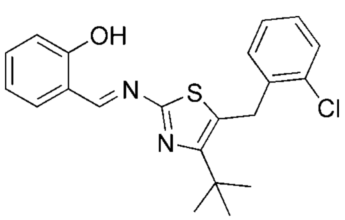
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.141; data-to-parameter ratio = 15.5.

The title compound, $C_{21}H_{21}ClN_2OS$, has been synthesized in a search for low-toxicity and potent fungicides. The phenol group is nearly coplanar with the thiazole ring, with a dihedral angle of 3.0 (2)°, and the 2-chlorobenzyl group is approximately perpendicular to the thiazole ring, the dihedral angle being 84.5 (2)°. Intramolecular O—H⋯N hydrogen bonding is observed in the structure.

Related literature

For general background, see: Hu *et al.* (2006, 2007); Shao *et al.* (2007).



Experimental

Crystal data

$C_{21}H_{21}ClN_2OS$
M_r = 384.91
Monoclinic, $P2_1/n$
a = 14.3753 (11) Å
b = 9.8665 (8) Å
c = 14.6565 (12) Å
β = 114.256 (1)°
V = 1895.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 173 (2) K
0.45 × 0.40 × 0.04 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.868, T_{max} = 0.988
8743 measured reflections
3712 independent reflections
2261 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.141
S = 1.03
3712 reflections
239 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1⋯N2	0.84	1.87	2.616 (3)	146

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2378).

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supplementary materials

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(*E*)-2-[4-*tert*-Butyl-5-(2-chlorobenzyl)thiazol-2-yliminomethyl]phenol

G. Cao, Y.-Q. Mang and A.-X. Hu

Comment

Imine derivatives are a kind of important agriculturally active compounds (Hu *et al.*, 2006). The bioassay results display that some of the 4-benzyl-5-triazole-2-imine derivatives possess a fungicidal activity against Physalospora piricola (Shao *et al.*, 2007). Herein we report the synthesis and crystal structure of teh title compound.

The molecular structure is illustrated in Fig. 1. Geometric parameters of the title compound are in the normal ranges. The length of C=N double bond is 1.286 (4) Å. The 4-hydroxyphenyl group is nearly co-planar with the thiazole ring with a dihedral angle of 3.0 (2)°, and the 2-chlorobenzyl group is approximately perpendicular to the thiazole ring, dihedral angle being 84.5 (2)°. The molecule is stabilized by intramolecular O–H···N hydrogen bonding (Table 1).

Experimental

4-Tert-butyl-5-(2-chlorobenzyl)thiazol-2-amine was prepared according to the literature method (Hu *et al.*, 2007). The title compound was prepared as follows: 1 mmol salicylal was dissolved in 5 ml of freshly dried alcohol and heated to 348 K. Then the above-prepared alcohol solution of 4-*tert*-butyl-5- (2-chlorobenzyl)thiazol-2-amine (1 mmol) was added dropwise and the resulting reaction mixture was stirred at this temperature for a further 5 h. The mixture was then cooled, and the yellow solid was separated by filtration and recrystallized from dried alcohol to give the desired (I). Yield: 77.3%.

Crystals suitable for X-ray analysis were obtained by slow evaporation from an alcohol solution.

Refinement

The hydroxy H atom was positioned geometrically (O—H = 0.84 Å) and refined as riding [U_{iso}(H) = 1.5 U_{eq}(O)]. Methyl H atoms were positioned geometrically (C—H = 0.98 Å) and torsion angles refined to fit the electron density [U_{iso}(H) = 1.5 U_{eq}(C)]. Other H atoms were placed in calculated positions (methylene C—H = 0.99 Å, C4—H4 = 0.95 Å and aromatic C—H = 0.95 Å) and refined as riding [U_{iso}(H) = 1.2 U_{eq}(C)].

Figures

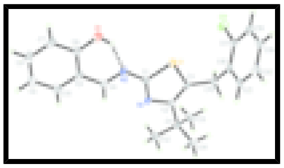

Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

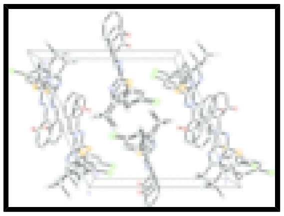

Fig. 2. The crystal packing for (I), with all H atoms omitted for clarity.

(*E*)-2-[4-*tert*-Butyl-5-(2-chlorobenzyl)thiazol-2-yliminomethyl]phenol

Crystal data

$C_{21}H_{21}ClN_2OS$	F_{000} = 808
M_r = 384.91	D_x = 1.349 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 415-416 K
Hall symbol: -P 2yn	Mo *K*α radiation λ = 0.71073 Å
a = 14.3753 (11) Å	Cell parameters from 2108 reflections
b = 9.8665 (8) Å	θ = 2.6–26.8°
c = 14.6565 (12) Å	μ = 0.32 mm^{-1}
β = 114.256 (1)°	*T* = 173 (2) K
V = 1895.3 (3) Å^3	Platelet, yellow
Z = 4	0.45 × 0.40 × 0.04 mm

Data collection

Bruker SMART 1000 CCD diffractometer	3712 independent reflections
Radiation source: fine-focus sealed tube	2261 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.046
T = 173(2) K	θ_{max} = 26.0°
ω scans	θ_{min} = 1.7°
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -16 \rightarrow 17$
T_{min} = 0.868, T_{max} = 0.988	$k = -8 \rightarrow 12$
8743 measured reflections	$l = -18 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained
$wR(F^2)$ = 0.141	$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2 + 0.7216P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
3712 reflections	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
239 parameters	$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

Special details

Experimental. Spectroscopic analysis: ^{1}H-NMR ($CDCl_3$, 400 MHz) (p.p.m.): 1.45(s, 9H, $(CH_3)_3$), 4.38(s, 2H, CH_2), 6.94(dd, J = 8.0 Hz, J = 8.0 Hz, 1H, 2-$HOC_6H_4$5-H), 6.99(d, J = 8.0 Hz, 1H, 2-$HOC_6H_4$3-H), 7.15–7.44(m, 6H, 2-ClC_6H_4, 2-$HOC_6H_4$4,6-H), 9.05(s, 1H, N=CH), 12.31(s, 1H, OH).

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

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}
Cl1	0.12770 (7)	0.39657 (10)	1.20048 (7)	0.0505 (3)
S1	0.26019 (6)	0.19364 (8)	1.07258 (6)	0.0321 (2)
C1	0.2842 (2)	0.0488 (3)	1.0210 (2)	0.0259 (7)
C2	0.1231 (2)	0.0851 (3)	0.9187 (2)	0.0236 (7)
C3	0.1380 (2)	0.1947 (3)	0.9809 (2)	0.0265 (7)
C4	0.4059 (2)	−0.1106 (3)	1.0279 (2)	0.0287 (7)
H4	0.3556	−0.1502	0.9693	0.034*
C5	0.5070 (2)	−0.1704 (3)	1.0723 (2)	0.0276 (7)
C6	0.5864 (2)	−0.1096 (3)	1.1541 (2)	0.0300 (7)
C7	0.6827 (2)	−0.1702 (3)	1.1944 (3)	0.0382 (8)
H7	0.7367	−0.1292	1.2495	0.046*
C8	0.6996 (3)	−0.2887 (3)	1.1549 (3)	0.0447 (9)
H8	0.7654	−0.3291	1.1828	0.054*
C9	0.6217 (3)	−0.3507 (4)	1.0742 (3)	0.0465 (10)
H9	0.6337	−0.4334	1.0477	0.056*
C10	0.5272 (3)	−0.2907 (3)	1.0336 (3)	0.0397 (8)
H10	0.4743	−0.3320	0.9777	0.048*
C11	0.0263 (2)	0.0488 (3)	0.8268 (2)	0.0287 (7)
C12	0.0344 (3)	−0.0939 (3)	0.7907 (3)	0.0483 (10)
H12A	0.0941	−0.0994	0.7747	0.072*
H12B	−0.0273	−0.1146	0.7308	0.072*
H12C	0.0416	−0.1594	0.8435	0.072*
C13	−0.0674 (2)	0.0514 (4)	0.8515 (3)	0.0456 (9)
H13A	−0.0587	−0.0150	0.9041	0.068*
H13B	−0.1285	0.0288	0.7914	0.068*
H13C	−0.0751	0.1421	0.8747	0.068*
C14	0.0127 (3)	0.1484 (4)	0.7429 (3)	0.0555 (11)

H14A	0.0048	0.2402	0.7642	0.083*
H14B	−0.0482	0.1240	0.6833	0.083*
H14C	0.0727	0.1452	0.7273	0.083*
C15	0.0666 (2)	0.3079 (3)	0.9796 (3)	0.0336 (8)
H15A	0.0310	0.2821	1.0222	0.040*
H15B	0.0144	0.3199	0.9104	0.040*
C16	0.1213 (2)	0.4412 (3)	1.0164 (2)	0.0297 (7)
C17	0.1528 (2)	0.4889 (3)	1.1124 (2)	0.0314 (7)
C18	0.2037 (2)	0.6114 (3)	1.1429 (3)	0.0354 (8)
H18	0.2245	0.6416	1.2100	0.043*
C19	0.2235 (2)	0.6878 (3)	1.0754 (3)	0.0400 (9)
H19	0.2584	0.7717	1.0956	0.048*
C20	0.1930 (3)	0.6442 (3)	0.9775 (3)	0.0425 (9)
H20	0.2063	0.6991	0.9310	0.051*
C21	0.1438 (2)	0.5230 (3)	0.9472 (3)	0.0371 (8)
H21	0.1247	0.4929	0.8804	0.045*
N1	0.20771 (18)	0.0024 (2)	0.94293 (18)	0.0265 (6)
N2	0.38305 (17)	−0.0053 (2)	1.06618 (19)	0.0275 (6)
O1	0.57396 (16)	0.0080 (2)	1.19436 (18)	0.0427 (6)
H1	0.5129	0.0329	1.1657	0.064*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0506 (6)	0.0546 (6)	0.0465 (6)	−0.0011 (4)	0.0202 (5)	0.0112 (5)
S1	0.0229 (4)	0.0304 (4)	0.0342 (5)	0.0003 (3)	0.0028 (3)	−0.0070 (4)
C1	0.0229 (16)	0.0256 (16)	0.0261 (17)	−0.0010 (12)	0.0068 (14)	0.0010 (13)
C2	0.0212 (15)	0.0223 (15)	0.0263 (17)	−0.0023 (12)	0.0085 (13)	0.0019 (13)
C3	0.0189 (15)	0.0271 (16)	0.0278 (17)	−0.0003 (12)	0.0039 (13)	0.0022 (14)
C4	0.0257 (16)	0.0293 (17)	0.0281 (17)	−0.0016 (13)	0.0081 (14)	0.0039 (14)
C5	0.0258 (16)	0.0286 (17)	0.0285 (18)	0.0017 (13)	0.0111 (14)	0.0063 (13)
C6	0.0245 (16)	0.0335 (18)	0.0314 (18)	0.0017 (13)	0.0109 (14)	0.0041 (14)
C7	0.0226 (17)	0.050 (2)	0.039 (2)	0.0031 (15)	0.0096 (16)	0.0104 (16)
C8	0.032 (2)	0.046 (2)	0.064 (3)	0.0133 (17)	0.0265 (19)	0.017 (2)
C9	0.044 (2)	0.0354 (19)	0.068 (3)	0.0103 (17)	0.030 (2)	0.0015 (19)
C10	0.0339 (19)	0.038 (2)	0.049 (2)	−0.0015 (15)	0.0187 (17)	−0.0037 (17)
C11	0.0230 (16)	0.0282 (16)	0.0279 (18)	0.0007 (13)	0.0034 (14)	−0.0019 (14)
C12	0.035 (2)	0.047 (2)	0.046 (2)	0.0033 (16)	0.0004 (17)	−0.0213 (18)
C13	0.0283 (19)	0.051 (2)	0.052 (2)	−0.0141 (16)	0.0107 (18)	−0.0192 (18)
C14	0.044 (2)	0.067 (3)	0.038 (2)	−0.0044 (19)	−0.0016 (18)	0.017 (2)
C15	0.0241 (16)	0.0268 (16)	0.045 (2)	−0.0009 (13)	0.0090 (15)	−0.0062 (15)
C16	0.0186 (15)	0.0249 (16)	0.038 (2)	0.0075 (12)	0.0040 (15)	0.0006 (14)
C17	0.0273 (17)	0.0289 (17)	0.0327 (19)	0.0066 (14)	0.0071 (15)	0.0040 (14)
C18	0.0269 (17)	0.0301 (18)	0.041 (2)	0.0040 (14)	0.0058 (15)	−0.0058 (16)
C19	0.0336 (19)	0.0311 (18)	0.049 (2)	−0.0024 (15)	0.0106 (17)	0.0005 (17)
C20	0.039 (2)	0.039 (2)	0.049 (2)	0.0040 (16)	0.0176 (18)	0.0127 (18)
C21	0.0263 (17)	0.0317 (19)	0.042 (2)	0.0059 (14)	0.0029 (16)	−0.0053 (15)
N1	0.0227 (13)	0.0241 (13)	0.0284 (15)	0.0027 (11)	0.0064 (12)	0.0027 (11)

N2	0.0207 (13)	0.0274 (14)	0.0301 (15)	0.0025 (11)	0.0061 (11)	0.0046 (12)
O1	0.0286 (13)	0.0470 (14)	0.0396 (15)	0.0040 (11)	0.0010 (11)	−0.0080 (12)

Geometric parameters (Å, °)

Cl1—C17	1.735 (3)	C11—C13	1.533 (4)
S1—C1	1.717 (3)	C12—H12A	0.9800
S1—C3	1.718 (3)	C12—H12B	0.9800
C1—N1	1.302 (4)	C12—H12C	0.9800
C1—N2	1.404 (4)	C13—H13A	0.9800
C2—C3	1.372 (4)	C13—H13B	0.9800
C2—N1	1.385 (3)	C13—H13C	0.9800
C2—C11	1.529 (4)	C14—H14A	0.9800
C3—C15	1.513 (4)	C14—H14B	0.9800
C4—N2	1.286 (4)	C14—H14C	0.9800
C4—C5	1.451 (4)	C15—C16	1.513 (4)
C4—H4	0.9500	C15—H15A	0.9900
C5—C10	1.397 (4)	C15—H15B	0.9900
C5—C6	1.405 (4)	C16—C17	1.372 (4)
C6—O1	1.347 (4)	C16—C21	1.433 (5)
C6—C7	1.397 (4)	C17—C18	1.388 (4)
C7—C8	1.371 (5)	C18—C19	1.364 (5)
C7—H7	0.9500	C18—H18	0.9500
C8—C9	1.392 (5)	C19—C20	1.385 (5)
C8—H8	0.9500	C19—H19	0.9500
C9—C10	1.373 (5)	C20—C21	1.368 (4)
C9—H9	0.9500	C20—H20	0.9500
C10—H10	0.9500	C21—H21	0.9500
C11—C14	1.522 (5)	O1—H1	0.8400
C11—C12	1.525 (4)		
C1—S1—C3	89.20 (14)	H12A—C12—H12C	109.5
N1—C1—N2	127.4 (3)	H12B—C12—H12C	109.5
N1—C1—S1	115.5 (2)	C11—C13—H13A	109.5
N2—C1—S1	117.2 (2)	C11—C13—H13B	109.5
C3—C2—N1	114.4 (3)	H13A—C13—H13B	109.5
C3—C2—C11	127.4 (3)	C11—C13—H13C	109.5
N1—C2—C11	118.2 (2)	H13A—C13—H13C	109.5
C2—C3—C15	130.8 (3)	H13B—C13—H13C	109.5
C2—C3—S1	110.2 (2)	C11—C14—H14A	109.5
C15—C3—S1	119.0 (2)	C11—C14—H14B	109.5
N2—C4—C5	121.4 (3)	H14A—C14—H14B	109.5
N2—C4—H4	119.3	C11—C14—H14C	109.5
C5—C4—H4	119.3	H14A—C14—H14C	109.5
C10—C5—C6	118.5 (3)	H14B—C14—H14C	109.5
C10—C5—C4	120.0 (3)	C3—C15—C16	112.8 (2)
C6—C5—C4	121.5 (3)	C3—C15—H15A	109.0
O1—C6—C7	118.1 (3)	C16—C15—H15A	109.0
O1—C6—C5	122.2 (3)	C3—C15—H15B	109.0
C7—C6—C5	119.7 (3)	C16—C15—H15B	109.0

C8—C7—C6	120.2 (3)	H15A—C15—H15B	107.8
C8—C7—H7	119.9	C17—C16—C21	117.2 (3)
C6—C7—H7	119.9	C17—C16—C15	124.6 (3)
C7—C8—C9	120.8 (3)	C21—C16—C15	118.2 (3)
C7—C8—H8	119.6	C16—C17—C18	122.5 (3)
C9—C8—H8	119.6	C16—C17—Cl1	120.0 (2)
C10—C9—C8	119.1 (3)	C18—C17—Cl1	117.5 (3)
C10—C9—H9	120.4	C19—C18—C17	119.1 (3)
C8—C9—H9	120.4	C19—C18—H18	120.4
C9—C10—C5	121.6 (3)	C17—C18—H18	120.4
C9—C10—H10	119.2	C18—C19—C20	120.6 (3)
C5—C10—H10	119.2	C18—C19—H19	119.7
C14—C11—C12	108.6 (3)	C20—C19—H19	119.7
C14—C11—C2	109.2 (3)	C21—C20—C19	120.6 (3)
C12—C11—C2	110.6 (2)	C21—C20—H20	119.7
C14—C11—C13	110.2 (3)	C19—C20—H20	119.7
C12—C11—C13	107.3 (3)	C20—C21—C16	120.0 (3)
C2—C11—C13	110.9 (3)	C20—C21—H21	120.0
C11—C12—H12A	109.5	C16—C21—H21	120.0
C11—C12—H12B	109.5	C1—N1—C2	110.7 (2)
H12A—C12—H12B	109.5	C4—N2—C1	119.5 (3)
C11—C12—H12C	109.5	C6—O1—H1	109.5

C3—S1—C1—N1	−1.1 (2)	C3—C2—C11—C13	−50.3 (4)
C3—S1—C1—N2	178.2 (2)	N1—C2—C11—C13	131.6 (3)
N1—C2—C3—C15	179.3 (3)	C2—C3—C15—C16	−146.9 (3)
C11—C2—C3—C15	1.2 (5)	S1—C3—C15—C16	33.1 (4)
N1—C2—C3—S1	−0.7 (3)	C3—C15—C16—C17	−96.4 (4)
C11—C2—C3—S1	−178.9 (2)	C3—C15—C16—C21	82.4 (3)
C1—S1—C3—C2	0.9 (2)	C21—C16—C17—C18	0.6 (4)
C1—S1—C3—C15	−179.1 (3)	C15—C16—C17—C18	179.3 (3)
N2—C4—C5—C10	175.1 (3)	C21—C16—C17—Cl1	179.6 (2)
N2—C4—C5—C6	−5.2 (5)	C15—C16—C17—Cl1	−1.7 (4)
C10—C5—C6—O1	178.5 (3)	C16—C17—C18—C19	0.0 (5)
C4—C5—C6—O1	−1.3 (5)	Cl1—C17—C18—C19	−179.1 (2)
C10—C5—C6—C7	−0.1 (5)	C17—C18—C19—C20	0.2 (5)
C4—C5—C6—C7	−179.8 (3)	C18—C19—C20—C21	−0.9 (5)
O1—C6—C7—C8	−178.9 (3)	C19—C20—C21—C16	1.5 (5)
C5—C6—C7—C8	−0.3 (5)	C17—C16—C21—C20	−1.3 (4)
C6—C7—C8—C9	−0.1 (5)	C15—C16—C21—C20	179.9 (3)
C7—C8—C9—C10	0.8 (5)	N2—C1—N1—C2	−178.3 (3)
C8—C9—C10—C5	−1.2 (5)	S1—C1—N1—C2	0.9 (3)
C6—C5—C10—C9	0.8 (5)	C3—C2—N1—C1	−0.1 (4)
C4—C5—C10—C9	−179.4 (3)	C11—C2—N1—C1	178.3 (3)
C3—C2—C11—C14	71.4 (4)	C5—C4—N2—C1	−179.7 (3)
N1—C2—C11—C14	−106.8 (3)	N1—C1—N2—C4	1.9 (5)
C3—C2—C11—C12	−169.2 (3)	S1—C1—N2—C4	−177.2 (2)
N1—C2—C11—C12	12.7 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.84	1.87	2.616 (3)	146

Fig. 1

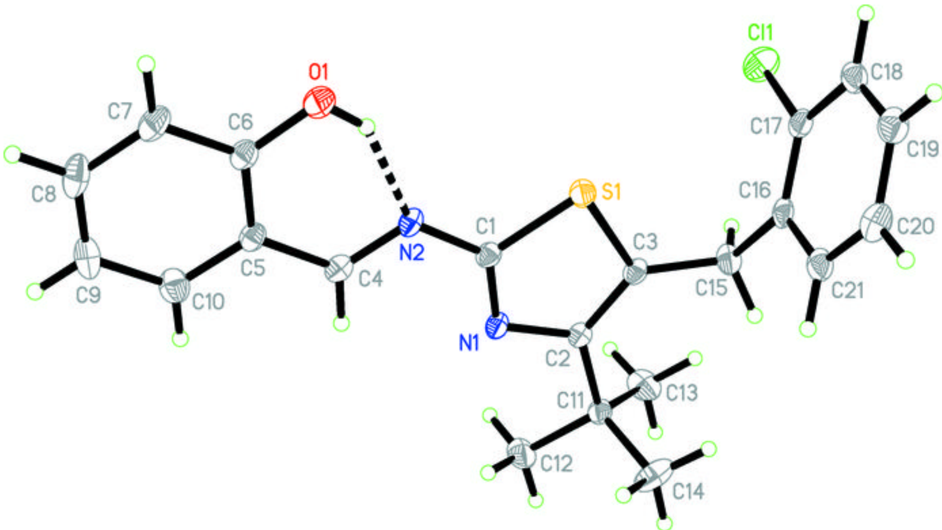
O1
C7
C6
C8
N2
C1
S1
C3
C5
C4
C9
C10
N1
C2
C11
C13
C12
C14
Cl1
C18
C17
C19
C16
C20
C15
C21

Fig. 2