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2-Amino-4-*tert*-butyl-5-(2-chlorobenzyl)thiazol-3-ium bromide

Gao Cao,[a] Ai-Xi Hu,[a]* Juan-Juan Xu[b] and Lin Xia[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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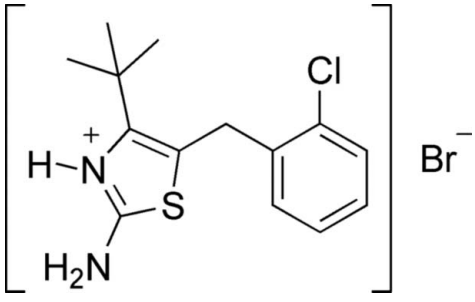
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.008 Å; disorder in main residue; R factor = 0.053; wR factor = 0.158; data-to-parameter ratio = 16.0.

As part of a search for potent fungicidal agents, the title compound, $C_{14}H_{18}ClN_2S^+\cdot Br^-$, has been synthesized. The dihedral angle between the planes of the thiazole and the chlorophenyl ring is 95.1 (2)°. The molecules are connecteded by N—H···Br hydrogen bonds. The *tert*-butyl group shows rotational disorder.

Related literature

For related literature, see: He *et al.* (2006); Marcantonio *et al.* (2002); Xu *et al.* (2007).



Experimental

Crystal data

$C_{14}H_{18}ClN_2S^+\cdot Br^-$ M_r = 361.72
Monoclinic, $P2_1/c$
a = 9.4439 (5) Å
b = 14.5569 (8) Å
c = 12.1926 (6) Å
β = 102.9880 (10)°
V = 1633.28 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.80 mm^{-1}
T = 173 (2) K
0.48 × 0.39 × 0.32 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.302, T_{max} = 0.407
10068 measured reflections
3203 independent reflections
2545 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.158
S = 1.05
3203 reflections
200 parameters
117 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···Br1^{i}	0.88	2.36	3.232 (4)	169
N2—H2A···Br1	0.88	2.54	3.314 (4)	147
N1—H1···Br1	0.88	2.50	3.262 (4)	146

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

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, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2341).

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supplementary materials

Acta Cryst. (2007). E**63**, o2534 [**doi:10.1107/S1600536807018065**]

2-Amino-4-*tert*-butyl-5-(2-chlorobenzyl)thiazol-3-ium bromide

G. Cao, A.-X. Hu, J.-J. Xu and L. Xia

Comment

2-Amino-4-arylthiazoles have been utilized extensively by chemists due to their pharmaceutical importance in drug design and extensive application in organic synthesis (Marcantonio *et al.*, 2002). The biological utility of 2-amino-4-arylthiazoles is wide-ranging, especially because of their antifungal activities. Two 2-Amino-4-arylthiazoles crystal structures were reported before (He *et al.*, 2006; Xu *et al.*, 2007). The title compound (I) was prepared as part of an ongoing investigation on the synthesis and structural properties of 2-amino-4-arylthiazole derivatives.

The dihedral angle between the chlorophenyl and thiazole ring planes is 95.1 (2)°. The molecules are linked by N–H···Br hydrogen bonds.

Experimental

1-(2-Chlorophenyl)-4,4-dimethylpentan-3-one (0.0067 mol) was dissolved in 267 ml e thanol and the mixture was stirred and heated to reflux. Cupric bromide (0.133 mol) was added to the reaction mixture in batches and the course of the reaction was followed by TLC analysis. After the reaction had finished, the mixture was filtered and concentrated in vacuo. The resulting residue was taken up in dichloromethane, washed with 10% hydrochloric acid, then washed with water until the solution was neutral, dried over anhydrous sodium sulfate and concentrated in vacuo to give 2-bromo-1-(2-chlorophenyl)-4,4-dimethylpentan-3-one, yield 90.8%. Then a solution of thiourea (0.03 mol) and the bromide (0.03 mol) in ethanol (82 ml) was refluxed for 9 h. The solvent was evaporated and the precipitate formed was filtered out, dried, giving white crystals of (I), yield 63.2%. The crystals suitable for X-ray structure determination were obtained by slow evaporation of an ethanol solution at room temperature.

Refinement

All H atoms were refined using a riding model, with N—H distances of 0.88 and C—H distances ranging from to 0.99 Å, and with $U_{iso}(H)=1.2U_{eq}(C, N)$, or $1.5U_{eq}(C_{methyl})$.

Figures

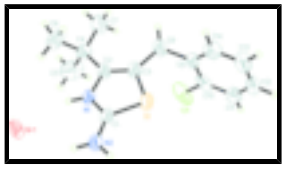

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids, H atoms are drawn as spheres of arbitrary radii. Only the major occupied sites of the disordered t-butyl group are shown.

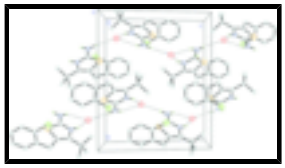

Fig. 2. The packing of (I), viewed down the *a* axis, showing the N—H···Br hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted. Only the major occupied sites of the disordered t-butyl group are shown.

2-Amino-4-tert-butyl-5-(2-chlorobenzyl)thiazol-3-ium bromide

Crystal data

$C_{14}H_{18}ClN_2S^+\cdot Br^-$	F_{000} = 736
M_r = 361.72	D_x = 1.471 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4663 reflections
a = 9.4439 (5) Å	θ = 2.2–26.9º
b = 14.5569 (8) Å	μ = 2.80 mm^{-1}
c = 12.1926 (6) Å	T = 173 (2) K
β = 102.9880 (10)º	Block, colorless
V = 1633.28 (15) Å^3	0.48 × 0.39 × 0.32 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD diffractometer	3203 independent reflections
Radiation source: fine-focus sealed tube	2545 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.023
T = 173(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→10
T_{min} = 0.302, T_{max} = 0.407	k = −17→17
10068 measured reflections	l = −14→15

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.053	$w = 1/[\sigma^2(F_o^2) + (0.0807P)^2 + 4.4972P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.158	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.05	$\Delta\rho_{max}$ = 2.10 e Å^{-3}
3203 reflections	$\Delta\rho_{min}$ = −0.83 e Å^{-3}
200 parameters	Extinction correction: none
117 restraints	

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

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. 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}	Occ. (<1)
Br1	0.70549 (6)	0.19049 (4)	0.14190 (4)	0.0487 (2)	
S1	0.41454 (15)	0.14640 (11)	0.47178 (11)	0.0561 (4)	
Cl1	−0.00232 (19)	0.19312 (14)	0.40805 (16)	0.0836 (6)	
C1	0.5088 (5)	0.1765 (3)	0.3711 (4)	0.0423 (11)	
C2	0.3359 (5)	0.0752 (3)	0.2738 (4)	0.0406 (10)	
C3	0.2996 (5)	0.0735 (4)	0.3747 (4)	0.0475 (12)	
C4	0.2775 (6)	0.0254 (4)	0.1637 (4)	0.0462 (11)	
C5	0.2212 (12)	0.0923 (6)	0.0703 (7)	0.091 (3)	0.852 (10)
H5A	0.1405	0.1275	0.0878	0.136*	0.852 (10)
H5B	0.1871	0.0588	−0.0004	0.136*	0.852 (10)
H5C	0.2993	0.1345	0.0625	0.136*	0.852 (10)
C6	0.4073 (9)	−0.0285 (6)	0.1333 (8)	0.075 (2)	0.852 (10)
H6A	0.4581	−0.0637	0.1990	0.112*	0.852 (10)
H6B	0.4749	0.0150	0.1111	0.112*	0.852 (10)
H6C	0.3699	−0.0707	0.0708	0.112*	0.852 (10)
C7	0.1650 (9)	−0.0479 (6)	0.1718 (7)	0.067 (2)	0.852 (10)
H7A	0.0774	−0.0185	0.1859	0.101*	0.852 (10)
H7B	0.2051	−0.0900	0.2337	0.101*	0.852 (10)
H7C	0.1401	−0.0824	0.1010	0.101*	0.852 (10)
C5A	0.112 (4)	0.066 (3)	0.122 (4)	0.069 (8)	0.148 (10)
H5AA	0.0729	0.0799	0.1884	0.104*	0.148 (10)
H5AB	0.0506	0.0200	0.0758	0.104*	0.148 (10)
H5AC	0.1142	0.1220	0.0785	0.104*	0.148 (10)
C6A	0.357 (4)	0.026 (3)	0.086 (3)	0.060 (8)	0.148 (10)
H6AA	0.3259	0.0769	0.0342	0.090*	0.148 (10)
H6AB	0.3425	−0.0323	0.0446	0.090*	0.148 (10)
H6AC	0.4594	0.0329	0.1231	0.090*	0.148 (10)
C7A	0.245 (5)	−0.076 (3)	0.205 (4)	0.064 (8)	0.148 (10)
H7AA	0.1514	−0.0756	0.2271	0.096*	0.148 (10)
H7AB	0.3222	−0.0931	0.2702	0.096*	0.148 (10)

H7AC	0.2422	−0.1197	0.1441	0.096*	0.148 (10)
C8	0.1870 (7)	0.0204 (4)	0.4199 (5)	0.0593 (15)	
H8A	0.0939	0.0208	0.3631	0.071*	
H8B	0.2190	−0.0442	0.4329	0.071*	
C9	0.1633 (5)	0.0608 (3)	0.5289 (4)	0.0444 (11)	
C10	0.0812 (5)	0.1407 (4)	0.5319 (5)	0.0507 (13)	
C11	0.0658 (6)	0.1785 (4)	0.6355 (5)	0.0529 (14)	
H11	0.0107	0.2328	0.6376	0.064*	
C12	0.1315 (6)	0.1350 (4)	0.7312 (5)	0.0559 (14)	
H12	0.1241	0.1603	0.8015	0.067*	
C13	0.2078 (7)	0.0564 (4)	0.7296 (5)	0.0600 (15)	
H13	0.2507	0.0263	0.7982	0.072*	
C14	0.2227 (6)	0.0206 (4)	0.6304 (5)	0.0537 (13)	
H14	0.2766	−0.0346	0.6311	0.064*	
N1	0.4537 (4)	0.1344 (3)	0.2742 (3)	0.0370 (8)	
H1	0.4889	0.1430	0.2140	0.044*	
N2	0.6226 (5)	0.2309 (3)	0.3875 (4)	0.0559 (12)	
H2A	0.6671	0.2412	0.3325	0.067*	
H2B	0.6545	0.2571	0.4535	0.067*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0529 (3)	0.0666 (4)	0.0289 (3)	−0.0152 (2)	0.0142 (2)	0.0046 (2)
S1	0.0563 (8)	0.0763 (10)	0.0442 (7)	−0.0278 (7)	0.0294 (6)	−0.0254 (7)
Cl1	0.0602 (9)	0.1074 (14)	0.0811 (12)	0.0073 (9)	0.0117 (8)	0.0524 (10)
C1	0.043 (3)	0.047 (3)	0.042 (3)	−0.010 (2)	0.019 (2)	−0.015 (2)
C2	0.035 (2)	0.049 (3)	0.041 (2)	−0.011 (2)	0.0145 (19)	−0.010 (2)
C3	0.047 (3)	0.056 (3)	0.043 (3)	−0.015 (2)	0.018 (2)	−0.015 (2)
C4	0.048 (3)	0.055 (3)	0.034 (2)	−0.010 (2)	0.0058 (19)	−0.008 (2)
C5	0.123 (7)	0.078 (5)	0.055 (4)	−0.003 (4)	−0.017 (4)	0.003 (4)
C6	0.065 (4)	0.083 (5)	0.078 (5)	−0.013 (3)	0.019 (4)	−0.044 (4)
C7	0.067 (4)	0.083 (5)	0.054 (4)	−0.034 (4)	0.019 (3)	−0.022 (3)
C5A	0.062 (9)	0.074 (11)	0.068 (12)	0.009 (9)	0.006 (8)	−0.009 (9)
C6A	0.063 (10)	0.067 (12)	0.052 (11)	−0.005 (8)	0.019 (8)	−0.007 (8)
C7A	0.070 (12)	0.061 (9)	0.062 (12)	−0.005 (8)	0.015 (9)	−0.003 (8)
C8	0.060 (3)	0.070 (4)	0.056 (3)	−0.024 (3)	0.031 (3)	−0.012 (3)
C9	0.038 (2)	0.050 (3)	0.052 (3)	−0.008 (2)	0.027 (2)	−0.006 (2)
C10	0.038 (3)	0.062 (3)	0.053 (3)	−0.010 (2)	0.012 (2)	0.022 (3)
C11	0.049 (3)	0.044 (3)	0.075 (4)	0.007 (2)	0.033 (3)	0.003 (3)
C12	0.064 (3)	0.064 (4)	0.048 (3)	−0.002 (3)	0.030 (3)	0.001 (3)
C13	0.061 (3)	0.071 (4)	0.051 (3)	0.006 (3)	0.019 (3)	0.012 (3)
C14	0.046 (3)	0.051 (3)	0.067 (4)	0.008 (2)	0.018 (3)	0.006 (3)
N1	0.039 (2)	0.044 (2)	0.0305 (18)	−0.0094 (17)	0.0129 (15)	−0.0109 (16)
N2	0.059 (3)	0.068 (3)	0.049 (2)	−0.034 (2)	0.029 (2)	−0.029 (2)

Geometric parameters (Å, °)

S1—C1	1.727 (5)	C5A—H5AB	0.9800

S1—C3	1.768 (5)	C5A—H5AC	0.9800
Cl1—C10	1.717 (5)	C6A—H6AA	0.9800
C1—N2	1.314 (6)	C6A—H6AB	0.9800
C1—N1	1.329 (6)	C6A—H6AC	0.9800
C2—C3	1.349 (6)	C7A—H7AA	0.9800
C2—N1	1.407 (6)	C7A—H7AB	0.9800
C2—C4	1.516 (6)	C7A—H7AC	0.9800
C3—C8	1.515 (7)	C8—C9	1.514 (7)
C4—C6A	1.33 (3)	C8—H8A	0.9900
C4—C5	1.502 (9)	C8—H8B	0.9900
C4—C7	1.525 (8)	C9—C14	1.369 (8)
C4—C6	1.568 (9)	C9—C10	1.403 (8)
C4—C7A	1.61 (3)	C10—C11	1.415 (8)
C4—C5A	1.64 (3)	C11—C12	1.349 (8)
C5—H5A	0.9800	C11—H11	0.9500
C5—H5B	0.9800	C12—C13	1.355 (8)
C5—H5C	0.9800	C12—H12	0.9500
C6—H6A	0.9800	C13—C14	1.353 (8)
C6—H6B	0.9800	C13—H13	0.9500
C6—H6C	0.9800	C14—H14	0.9500
C7—H7A	0.9800	N1—H1	0.8800
C7—H7B	0.9800	N2—H2A	0.8800
C7—H7C	0.9800	N2—H2B	0.8800
C5A—H5AA	0.9800		
C1—S1—C3	90.8 (2)	C4—C5A—H5AB	109.5
N2—C1—N1	123.8 (4)	H5AA—C5A—H5AB	109.5
N2—C1—S1	125.4 (4)	C4—C5A—H5AC	109.5
N1—C1—S1	110.7 (3)	H5AA—C5A—H5AC	109.5
C3—C2—N1	111.7 (4)	H5AB—C5A—H5AC	109.5
C3—C2—C4	133.1 (4)	C4—C6A—H6AA	109.5
N1—C2—C4	115.2 (4)	C4—C6A—H6AB	109.5
C2—C3—C8	133.1 (5)	H6AA—C6A—H6AB	109.5
C2—C3—S1	110.9 (4)	C4—C6A—H6AC	109.5
C8—C3—S1	116.0 (4)	H6AA—C6A—H6AC	109.5
C6A—C4—C5	68 (2)	H6AB—C6A—H6AC	109.5
C6A—C4—C2	118.5 (18)	C4—C7A—H7AA	109.5
C5—C4—C2	111.0 (5)	C4—C7A—H7AB	109.5
C6A—C4—C7	124.1 (18)	H7AA—C7A—H7AB	109.5
C5—C4—C7	111.7 (6)	C4—C7A—H7AC	109.5
C2—C4—C7	113.4 (5)	H7AA—C7A—H7AC	109.5
C5—C4—C6	107.9 (7)	H7AB—C7A—H7AC	109.5
C2—C4—C6	107.5 (5)	C9—C8—C3	112.1 (4)
C7—C4—C6	104.9 (6)	C9—C8—H8A	109.2
C6A—C4—C7A	114 (2)	C3—C8—H8A	109.2
C5—C4—C7A	140.6 (19)	C9—C8—H8B	109.2
C2—C4—C7A	102.4 (17)	C3—C8—H8B	109.2
C6—C4—C7A	80.2 (17)	H8A—C8—H8B	107.9
C6A—C4—C5A	115 (2)	C14—C9—C10	116.6 (5)
C5—C4—C5A	51.9 (16)	C14—C9—C8	121.0 (5)

C2—C4—C5A	103.4 (16)	C10—C9—C8	122.4 (5)
C7—C4—C5A	69.0 (17)	C9—C10—C11	120.9 (5)
C6—C4—C5A	148.1 (16)	C9—C10—Cl1	119.5 (4)
C7A—C4—C5A	101 (2)	C11—C10—Cl1	119.6 (4)
C4—C5—H5A	109.5	C12—C11—C10	118.1 (5)
C4—C5—H5B	109.5	C12—C11—H11	121.0
H5A—C5—H5B	109.5	C10—C11—H11	121.0
C4—C5—H5C	109.5	C11—C12—C13	121.8 (5)
H5A—C5—H5C	109.5	C11—C12—H12	119.1
H5B—C5—H5C	109.5	C13—C12—H12	119.1
C4—C6—H6A	109.5	C14—C13—C12	120.0 (6)
C4—C6—H6B	109.5	C14—C13—H13	120.0
H6A—C6—H6B	109.5	C12—C13—H13	120.0
C4—C6—H6C	109.5	C13—C14—C9	122.7 (5)
H6A—C6—H6C	109.5	C13—C14—H14	118.7
H6B—C6—H6C	109.5	C9—C14—H14	118.7
C4—C7—H7A	109.5	C1—N1—C2	115.9 (4)
C4—C7—H7B	109.5	C1—N1—H1	122.1
H7A—C7—H7B	109.5	C2—N1—H1	122.1
C4—C7—H7C	109.5	C1—N2—H2A	120.0
H7A—C7—H7C	109.5	C1—N2—H2B	120.0
H7B—C7—H7C	109.5	H2A—N2—H2B	120.0
C4—C5A—H5AA	109.5		
C3—S1—C1—N2	−177.2 (5)	C2—C3—C8—C9	−165.2 (6)
C3—S1—C1—N1	0.5 (4)	S1—C3—C8—C9	17.5 (7)
N1—C2—C3—C8	−177.7 (6)	C3—C8—C9—C14	−102.7 (6)
C4—C2—C3—C8	0.9 (11)	C3—C8—C9—C10	76.8 (7)
N1—C2—C3—S1	−0.3 (6)	C14—C9—C10—C11	1.9 (7)
C4—C2—C3—S1	178.3 (5)	C8—C9—C10—C11	−177.6 (5)
C1—S1—C3—C2	−0.1 (5)	C14—C9—C10—Cl1	−177.7 (4)
C1—S1—C3—C8	177.8 (5)	C8—C9—C10—Cl1	2.8 (7)
C3—C2—C4—C6A	−165 (2)	C9—C10—C11—C12	−0.4 (8)
N1—C2—C4—C6A	14 (2)	Cl1—C10—C11—C12	179.3 (4)
C3—C2—C4—C5	119.8 (8)	C10—C11—C12—C13	−1.5 (9)
N1—C2—C4—C5	−61.6 (7)	C11—C12—C13—C14	1.7 (9)
C3—C2—C4—C7	−6.8 (10)	C12—C13—C14—C9	0.0 (9)
N1—C2—C4—C7	171.7 (6)	C10—C9—C14—C13	−1.7 (8)
C3—C2—C4—C6	−122.3 (7)	C8—C9—C14—C13	177.8 (5)
N1—C2—C4—C6	56.2 (7)	N2—C1—N1—C2	177.0 (5)
C3—C2—C4—C7A	−38.8 (19)	S1—C1—N1—C2	−0.8 (6)
N1—C2—C4—C7A	139.8 (18)	C3—C2—N1—C1	0.7 (7)
C3—C2—C4—C5A	65.8 (19)	C4—C2—N1—C1	−178.2 (4)
N1—C2—C4—C5A	−115.6 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···Br1^{i}	0.88	2.36	3.232 (4)	169
N2—H2A···Br1	0.88	2.54	3.314 (4)	147

N1—H1···Br1	0.88	2.50	3.262 (4)	146

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

Fig. 1

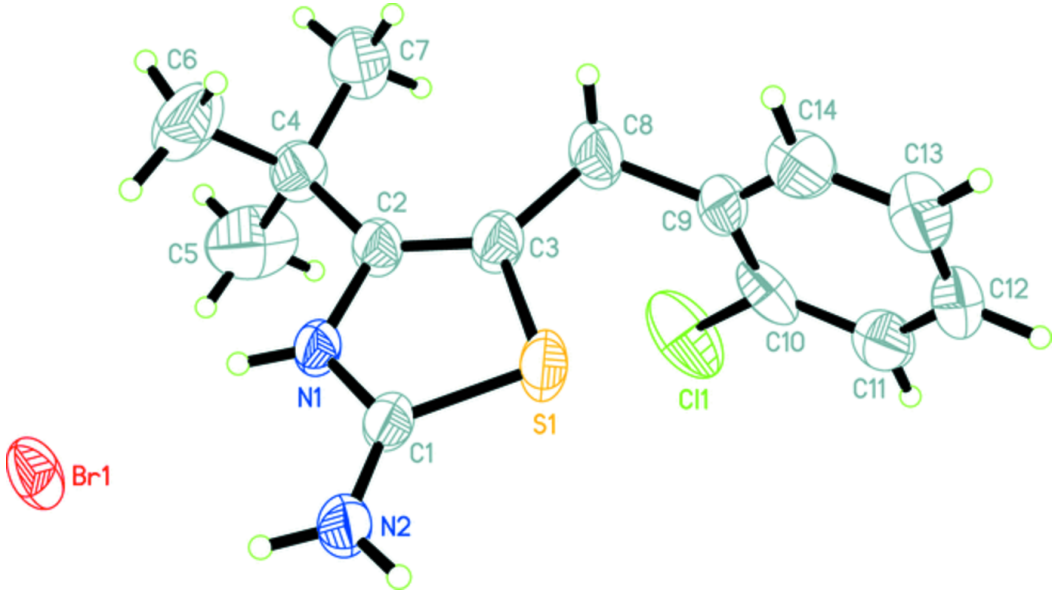

Fig. 2