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N-[4-(3-Chlorobenzyloxy)phenyl]-4,5-dihydrothiazol-2-amine

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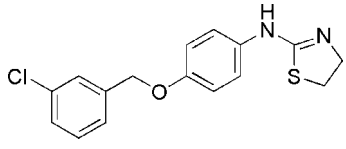
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.140; data-to-parameter ratio = 14.3.

The title compound, $C_{16}H_{15}ClN_2OS$, has been designed and synthesized as a potential herbicide. The benzene rings are approximately perpendicular to one another, making a dihedral angle of 95°. The thiazoline ring is not quite planar, with a mean deviation of 0.076 Å from the least-squares plane through the five ring atoms. Intermolecular N—H···N hydrogen bonds link the molecules into pairs around a center of symmetry. No other obvious intermolecular interactions are observed in the crystal structure.

Related literature

For related literature, see: Carey (2000); Wang *et al.* (2006); Xue *et al.* (2006); Morales-Bonilla *et al.* (2006); Van Muijlwijk-Koezen *et al.* (2001); Gao & Han (2002); Luo *et al.* (2006).



Experimental

Crystal data

$C_{16}H_{15}ClN_2OS$
M_r = 318.81
Monoclinic, $P2_1/c$
a = 12.134 (2) Å
b = 16.931 (3) Å
c = 7.8643 (15) Å
β = 106.655 (3)°
V = 1547.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 294 (2) K
0.18 × 0.16 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.935, T_{max} = 0.963
7919 measured reflections
2734 independent reflections
1886 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.140
S = 1.05
2734 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.86	2.09	2.934 (3)	166

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

The X-ray data were collected at Nankai University. This project was supported by the China 973 Program (2003CB114406).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2175).

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supplementary materials

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N-[4-(3-Chlorobenzyloxy)phenyl]-4,5-dihydrothiazol-2-amine

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Comment

Thiazole and its derivatives are often used to construct bioactive molecules, such as antibiotics (Morales-Bonilla *et al.*, 2006), anti-inflammatory drugs (Van Muijlwijk-Koezen *et al.*, 2001), anit-HIV drugs (Gao & Han, 2002) and agrochemicals (fungicides, herbicides, plant growth regulators and antiphytoviral agents) (Luo *et al.*, 2006). Using a *m*-Chlorobenzenyl group, instead of a 4-substituted benzoxylamidine, could increase inhibitory activity to the KARI enzyme in herbs (Wang *et al.*, 2006). Thus the title compound was designed and synthesized.

The molecular structure of (I) is shown in Fig. 1. The structure consists of a *m*-Cl-benzene ring (plane 1), a second benzene ring (plane 2) and as thiazolidine ring (plane 3). Plane 1 and 2 approximately perpendicular to one another with a dihedral angle of 95°. Plane 3 is not quite planar with a mean deviation from plane of 0.076Å for the 5 ring atoms. The bond length of N(1)—C(14) [1.28 Å] is much shorter than a normal C—N bond [1.47 Å] (Carey, 2000), but close to a C—N double bond [1.27 Å] (Xue *et al.*, 2006). Besides, the N(2)—C(14) [1.35 Å] is longer than a normal C—N double bond suggesting that N(1)—C(14)—N (2) is a conjugated system. In addition, the bond length of N(1)—C(11) [1.45 Å] is also a little shorter than the normal C—N single bond, which indicates that N(1)—C(14)—N(2) is conjugated with the neighboring benzene ring.

There is an intermolecular N—H···N hydrogen bond between the hydrogen atom of the N—H group of the amine moiety and the nitrogen atom of thiazoline group which link the molecules into pairs around a center of symmetry. No other obvious intermolecular interactions are observed in the crystal structure. Thus, these hydrogen bonds which link molecules into pairs are the main factors stablizing the crystal structure(Fig.2).

Experimental

m-Chlorobenzyl chloride (2.66 g, 0.016 mol), *p*-nitrophenol (2.09 g, 0.015 mol), potassium carbonate (2.96 g, 0.02 mol) and potassium iodide (0.2 g) were refluxed in ethanol for 8 h with TLC monitoring. Thereafter the mixture was cooled to room temperature and filtered. The resulting solid was washed by 10% sodium hydroxide and water and dried to give 4-nitrophenyl-*m*-chlorobenzyl ether (compound 1).

Compound 1 (18.45 g, 0.07 mol), 75 ml 80% hydrazine hydrate and 0.5 g Raney Ni were then refluxed in 100 ml e thanol for 1 h with TLC monitoring. The hot mixture was filtered and a white solid precipitated at once in the filtrate. The solid was filtered and washed with ethanol-water (1:1) for 3 three times, dried to give 4-(*m*-chlorobenzyloxyl) aniline (compound 2).

2-Iodo-2-methylsulfanyl-thiazolidine (0.78 g, 3 mmol) was then treated with compound 2(0.97 g, 3.6 mmol) in ethanol with refluxing for 5 h. The mixture was cooled to room temperature and then basified with 5 ml 10% sodium hydroxide aqueous solution. The resulting precipitate was filtered, washed with water and dried. The crude product was recrystallized from dichloromethane-petroleum ether (1:10) to give the title compound(0.7 g, 66.3%, m.p. 121 °C). Single crystals were obtained by slow evaporaton of a slution in dichloromethane-petroleum ether. ^{1}H NMR ($CDCl_3$): δ 7.44 (s, 1H, Ph—H),

7.30(m, 3H, Ph—H), 7.05(d, *J*=8.7 Hz, 2H, Ph—H),6.89(d, *J*=9.0 Hz, 2H, Ph—H), 5.00(s, 2H,OCH_2), 3.78–3.81(t, *J*=6.0 Hz, 2H, thiazolidine-H) 3.28–3.32(t, *J*=6.0 Hz, 2H, thiazolidine-H); FTMS: Calcd.: m/*z* 319.0666. Found: m/*z* 319.0672.

Refinement

All C—H H atoms were placed in calculated positions[C—H = 0.95, 0.99 and 1.00Å for phenyl, methylene and methine H atoms, respectively] and included in the refinement using a riding model, with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(methyl C)·The H atom of N—H were located in difference Fourier maps and refined freely with isotropic displacement parameters.

Figures

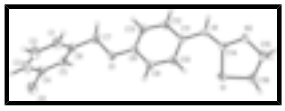

Fig. 1. The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level.

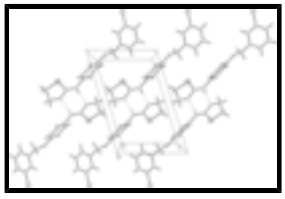

Fig. 2. The crystal packing of I, showing the N—H–N hydrogen bonds (dashed lines).

N-[4-(3-Chlorobenzyloxy)phenyl]-4,5-dihydrothiazol-2-amine

Crystal data

$C_{16}H_{15}ClN_2OS$	D_x = 1.368 Mg m^{-3}
M_r = 318.81	Melting point: 121 K
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.134 (2) Å	Cell parameters from 2358 reflections
b = 16.931 (3) Å	θ = 3.0–25.7º
c = 7.8643 (15) Å	μ = 0.38 mm^{-1}
β = 106.655 (3)º	*T* = 294 (2) K
V = 1547.9 (5) Å^3	Stick, light yellow
Z = 4	0.18 × 0.16 × 0.10 mm
F_{000} = 664	

Data collection

Bruker SMART CCD area-detector diffractometer	2734 independent reflections
Radiation source: fine-focus sealed tube	1886 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 294(2) K	θ_{max} = 25.0º
phi and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	*h* = −14→14

T_{min} = 0.935, T_{max} = 0.963
7919 measured reflections
k = −20→20
l = −7→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.140
S = 1.05
2734 reflections
191 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 1.1051P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}
Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.018 (2)

Special details

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	−0.44037 (7)	0.16311 (7)	−0.19685 (14)	0.0754 (4)
S1	0.28855 (8)	0.14421 (7)	1.12062 (12)	0.0750 (4)
N1	0.35478 (19)	0.04645 (14)	0.8894 (3)	0.0445 (6)
H1	0.4009	0.0103	0.8742	0.053*
O1	0.00845 (19)	0.12883 (12)	0.2774 (3)	0.0587 (6)
C14	0.3745 (2)	0.07591 (17)	1.0451 (4)	0.0392 (7)
C10	0.2216 (2)	0.14505 (17)	0.7055 (4)	0.0433 (7)
H10	0.2510	0.1851	0.7868	0.052*
C11	0.2640 (2)	0.06825 (17)	0.7411 (4)	0.0379 (7)
C8	0.0915 (2)	0.10457 (17)	0.4272 (4)	0.0434 (7)
N2	0.4668 (2)	0.05489 (16)	1.1801 (3)	0.0549 (7)
C6	−0.1048 (3)	0.11467 (17)	−0.0210 (4)	0.0436 (7)
C9	0.1365 (3)	0.16218 (17)	0.5513 (4)	0.0452 (7)
H9	0.1091	0.2136	0.5307	0.054*

C12	0.2184 (3)	0.01120 (17)	0.6141 (4)	0.0473 (8)
H12	0.2460	−0.0402	0.6335	0.057*
C5	−0.2217 (3)	0.11745 (17)	−0.0389 (4)	0.0469 (8)
H5	−0.2514	0.0920	0.0431	0.056*
C13	0.1330 (3)	0.02835 (18)	0.4595 (4)	0.0521 (8)
H13	0.1037	−0.0114	0.3773	0.062*
C4	−0.2938 (3)	0.15819 (18)	−0.1791 (4)	0.0488 (8)
C1	−0.0635 (3)	0.15127 (19)	−0.1474 (5)	0.0554 (8)
H1A	0.0147	0.1494	−0.1374	0.066*
C2	−0.1371 (3)	0.1906 (2)	−0.2883 (5)	0.0648 (10)
H2	−0.1081	0.2145	−0.3730	0.078*
C3	−0.2528 (3)	0.1949 (2)	−0.3049 (5)	0.0606 (9)
H3	−0.3023	0.2220	−0.3991	0.073*
C16	0.3788 (3)	0.1378 (3)	1.3470 (5)	0.0721 (11)
H16A	0.3954	0.1902	1.3981	0.087*
H16B	0.3408	0.1076	1.4186	0.087*
C15	0.4866 (3)	0.0981 (3)	1.3413 (5)	0.0823 (13)
H15A	0.5463	0.1371	1.3490	0.099*
H15B	0.5123	0.0625	1.4416	0.099*
C7	−0.0250 (3)	0.07311 (19)	0.1341 (4)	0.0525 (8)
H7A	−0.0634	0.0282	0.1686	0.063*
H7B	0.0422	0.0541	0.1032	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0462 (5)	0.0977 (8)	0.0723 (7)	0.0030 (5)	0.0012 (4)	−0.0024 (5)
S1	0.0659 (6)	0.1079 (8)	0.0439 (5)	0.0472 (6)	0.0038 (4)	−0.0130 (5)
N1	0.0391 (13)	0.0471 (14)	0.0409 (14)	0.0151 (11)	0.0010 (11)	−0.0045 (12)
O1	0.0648 (14)	0.0523 (13)	0.0406 (12)	0.0181 (11)	−0.0141 (11)	−0.0089 (10)
C14	0.0367 (15)	0.0397 (16)	0.0394 (17)	0.0025 (12)	0.0079 (13)	0.0000 (13)
C10	0.0464 (17)	0.0382 (16)	0.0390 (16)	0.0012 (13)	0.0023 (13)	−0.0048 (13)
C11	0.0339 (14)	0.0432 (16)	0.0342 (15)	0.0062 (12)	0.0060 (12)	−0.0009 (13)
C8	0.0403 (16)	0.0458 (17)	0.0372 (16)	0.0065 (13)	0.0001 (13)	−0.0010 (14)
N2	0.0509 (16)	0.0669 (18)	0.0353 (14)	0.0185 (13)	−0.0065 (12)	−0.0094 (13)
C6	0.0468 (18)	0.0367 (16)	0.0381 (16)	−0.0022 (13)	−0.0023 (14)	−0.0063 (13)
C9	0.0496 (17)	0.0384 (16)	0.0396 (17)	0.0086 (14)	0.0001 (14)	−0.0013 (14)
C12	0.0528 (18)	0.0374 (16)	0.0435 (17)	0.0105 (14)	0.0005 (14)	−0.0025 (14)
C5	0.0519 (19)	0.0472 (17)	0.0345 (16)	−0.0049 (14)	0.0012 (14)	0.0011 (14)
C13	0.0572 (19)	0.0427 (17)	0.0444 (18)	0.0057 (15)	−0.0044 (15)	−0.0097 (15)
C4	0.0445 (17)	0.0481 (18)	0.0453 (18)	−0.0035 (14)	−0.0010 (14)	−0.0038 (15)
C1	0.0480 (18)	0.054 (2)	0.058 (2)	−0.0083 (15)	0.0055 (16)	0.0008 (17)
C2	0.068 (2)	0.066 (2)	0.057 (2)	−0.0122 (19)	0.0130 (19)	0.0147 (18)
C3	0.062 (2)	0.056 (2)	0.050 (2)	−0.0051 (17)	−0.0047 (17)	0.0134 (17)
C16	0.062 (2)	0.108 (3)	0.0409 (19)	0.024 (2)	0.0048 (17)	−0.013 (2)
C15	0.082 (3)	0.108 (3)	0.043 (2)	0.044 (2)	−0.0055 (18)	−0.020 (2)
C7	0.0559 (19)	0.0496 (18)	0.0408 (18)	0.0037 (15)	−0.0040 (15)	−0.0062 (15)

Geometric parameters (Å, °)

Cl1—C4	1.745 (3)	C9—H9	0.9300
S1—C14	1.770 (3)	C12—C13	1.383 (4)
S1—C16	1.807 (3)	C12—H12	0.9300
N1—C14	1.280 (4)	C5—C4	1.380 (4)
N1—C11	1.405 (3)	C5—H5	0.9300
N1—H1	0.8600	C13—H13	0.9300
O1—C8	1.375 (3)	C4—C3	1.377 (5)
O1—C7	1.436 (4)	C1—C2	1.379 (5)
C14—N2	1.351 (3)	C1—H1A	0.9300
C10—C9	1.379 (4)	C2—C3	1.374 (5)
C10—C11	1.397 (4)	C2—H2	0.9300
C10—H10	0.9300	C3—H3	0.9300
C11—C12	1.386 (4)	C16—C15	1.483 (5)
C8—C9	1.377 (4)	C16—H16A	0.9700
C8—C13	1.382 (4)	C16—H16B	0.9700
N2—C15	1.423 (4)	C15—H15A	0.9700
C6—C1	1.381 (4)	C15—H15B	0.9700
C6—C5	1.386 (4)	C7—H7A	0.9700
C6—C7	1.498 (4)	C7—H7B	0.9700
C14—S1—C16	92.43 (15)	C12—C13—H13	120.0
C14—N1—C11	125.4 (2)	C3—C4—C5	121.5 (3)
C14—N1—H1	117.3	C3—C4—Cl1	119.4 (2)
C11—N1—H1	117.3	C5—C4—Cl1	119.1 (3)
C8—O1—C7	116.7 (2)	C2—C1—C6	120.7 (3)
N1—C14—N2	122.4 (3)	C2—C1—H1A	119.6
N1—C14—S1	127.5 (2)	C6—C1—H1A	119.6
N2—C14—S1	110.1 (2)	C3—C2—C1	120.7 (3)
C9—C10—C11	120.8 (3)	C3—C2—H2	119.7
C9—C10—H10	119.6	C1—C2—H2	119.7
C11—C10—H10	119.6	C2—C3—C4	118.6 (3)
C12—C11—C10	117.2 (3)	C2—C3—H3	120.7
C12—C11—N1	118.1 (2)	C4—C3—H3	120.7
C10—C11—N1	124.5 (3)	C15—C16—S1	106.8 (2)
O1—C8—C9	116.1 (3)	C15—C16—H16A	110.4
O1—C8—C13	125.1 (3)	S1—C16—H16A	110.4
C9—C8—C13	118.8 (3)	C15—C16—H16B	110.4
C14—N2—C15	117.1 (3)	S1—C16—H16B	110.4
C1—C6—C5	118.9 (3)	H16A—C16—H16B	108.6
C1—C6—C7	120.9 (3)	N2—C15—C16	109.6 (3)
C5—C6—C7	120.2 (3)	N2—C15—H15A	109.8
C8—C9—C10	121.3 (3)	C16—C15—H15A	109.8
C8—C9—H9	119.4	N2—C15—H15B	109.8
C10—C9—H9	119.4	C16—C15—H15B	109.8
C13—C12—C11	122.1 (3)	H15A—C15—H15B	108.2
C13—C12—H12	119.0	O1—C7—C6	107.6 (2)
C11—C12—H12	119.0	O1—C7—H7A	110.2

C4—C5—C6	119.6 (3)	C6—C7—H7A	110.2
C4—C5—H5	120.2	O1—C7—H7B	110.2
C6—C5—H5	120.2	C6—C7—H7B	110.2
C8—C13—C12	119.9 (3)	H7A—C7—H7B	108.5
C8—C13—H13	120.0		
C11—N1—C14—N2	−176.8 (3)	C7—C6—C5—C4	177.8 (3)
C11—N1—C14—S1	5.9 (5)	O1—C8—C13—C12	178.9 (3)
C16—S1—C14—N1	174.1 (3)	C9—C8—C13—C12	0.0 (5)
C16—S1—C14—N2	−3.5 (3)	C11—C12—C13—C8	0.6 (5)
C9—C10—C11—C12	1.1 (4)	C6—C5—C4—C3	1.5 (5)
C9—C10—C11—N1	176.1 (3)	C6—C5—C4—Cl1	−178.5 (2)
C14—N1—C11—C12	−148.8 (3)	C5—C6—C1—C2	0.6 (5)
C14—N1—C11—C10	36.2 (5)	C7—C6—C1—C2	−178.9 (3)
C7—O1—C8—C9	169.6 (3)	C6—C1—C2—C3	0.7 (5)
C7—O1—C8—C13	−9.3 (5)	C1—C2—C3—C4	−0.8 (5)
N1—C14—N2—C15	173.1 (3)	C5—C4—C3—C2	−0.3 (5)
S1—C14—N2—C15	−9.1 (4)	Cl1—C4—C3—C2	179.8 (3)
O1—C8—C9—C10	−179.0 (3)	C14—S1—C16—C15	13.9 (3)
C13—C8—C9—C10	0.0 (5)	C14—N2—C15—C16	20.2 (5)
C11—C10—C9—C8	−0.5 (5)	S1—C16—C15—N2	−20.7 (5)
C10—C11—C12—C13	−1.1 (5)	C8—O1—C7—C6	−173.4 (3)
N1—C11—C12—C13	−176.5 (3)	C1—C6—C7—O1	92.5 (3)
C1—C6—C5—C4	−1.7 (4)	C5—C6—C7—O1	−87.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.86	2.09	2.934 (3)	166

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

Fig. 1

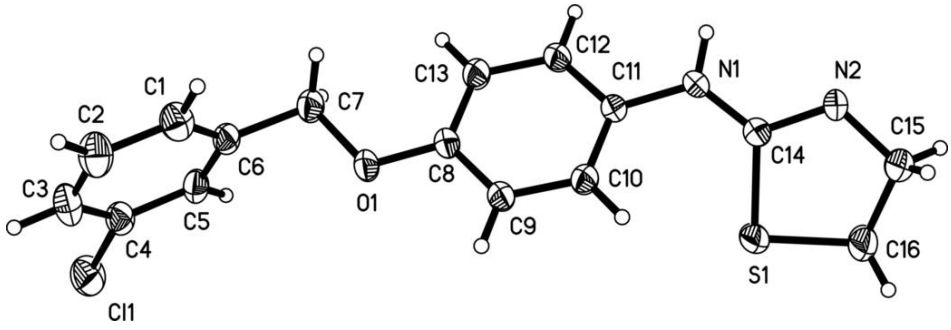
C12
C13
C11
N1
N2
C1
C7
C15
C2
C14
C6
C8
C10
C3
O1
C5
C9
C4
S1
C16
Cl1

Fig. 2