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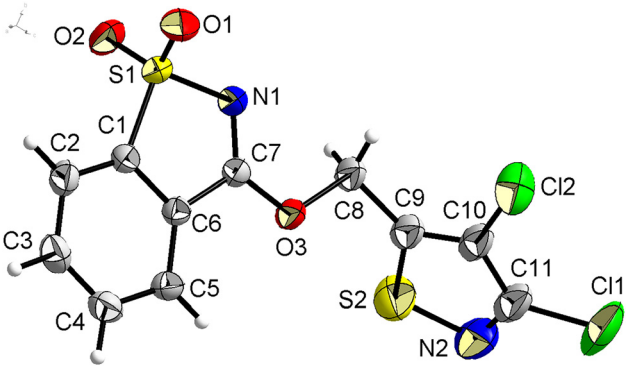
Crystal structure of 3-((3,4-dichloroisothiazol-5-yl)methoxy)benzo[*d*] isothiazole 1,1-dioxide, $C_{11}H_6Cl_2N_2O_3S_2$



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Abstract

$C_{11}H_6Cl_2N_2O_3S_2$, triclinic, $P\bar{1}$ (no. 2), a = 6.974(3) Å, b = 8.132(3) Å, c = 12.349(5) Å, α = 86.123(4)°, β = 78.299(4)°, γ = 85.715(4)°, V = 682.9(4) Å^3, Z = 2, $R_{gt}(F)$ = 0.0410, $wR_{ref}(F^2)$ = 0.1058, T = 296(2) K.

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.22 × 0.16 × 0.12 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.79 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.5°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5210, 2527, 0.017
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2302
$N(param)_{refined}$:	182
Programs:	Bruker [1], SHELX [2, 3], Diamond [4]

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of materials

Under stirring, add (3,4-dichloroisothiazol-5-yl)methanol and 3-chlorobenzo[*d*]isothiazole-1,1-dioxide 1:1 into the round-bottomed flask in turn, add an appropriate amount of acetonitrile and triethylamine, and react at room temperature for 5 h. Crystals of the title compound were obtained by slow evaporation of 3-((3,4-dichloroisothiazol-5-yl)methoxy)benzo[*d*] isothiazole 1,1-dioxide in ethyl acetate within one week.

Experimental details

All H atoms were included in calculated positions and refined as riding atoms, with C–H = 0.90–0.97 Å with U_{iso}(H) = 1.5 U_{eq}(C) for methyl H atoms and 1.2 U_{eq}(C) for all other H atoms.

Comment

In agricultural production, plant fungicides are widely used to control crop diseases [5, 6]. However, traditional plant fungicides generally pollute the environment [7],

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2730 (3)	0.6054 (3)	−0.10741 (18)	0.0323 (5)
C2	0.2773 (4)	0.4946 (3)	−0.1873 (2)	0.0410 (5)
H2	0.2900	0.5284	−0.2618	0.049*
C3	0.2616 (4)	0.3298 (3)	−0.1513 (2)	0.0459 (6)
H3	0.2641	0.2511	−0.2029	0.055*
C4	0.2421 (4)	0.2798 (3)	−0.0402 (2)	0.0437 (6)
H4	0.2334	0.1683	−0.0188	0.052*
C5	0.2356 (3)	0.3940 (3)	0.0396 (2)	0.0368 (5)
H5	0.2209	0.3612	0.1143	0.044*
C6	0.2517 (3)	0.5572 (3)	0.00376 (17)	0.0299 (4)
C7	0.2475 (3)	0.7053 (3)	0.06823 (17)	0.0312 (5)
C8	0.2138 (4)	0.8298 (3)	0.23837 (19)	0.0415 (6)
H8A	0.1102	0.9077	0.2215	0.050*
H8B	0.3372	0.8828	0.2197	0.050*
C9	0.1716 (4)	0.7736 (3)	0.3580 (2)	0.0443 (6)
C10	0.0039 (4)	0.7969 (3)	0.4340 (2)	0.0476 (6)
C11	0.0230 (6)	0.7247 (4)	0.5385 (2)	0.0603 (8)
Cl1	−0.16202 (18)	0.73856 (15)	0.65283 (7)	0.0970 (4)
Cl2	−0.20521 (12)	0.90304 (12)	0.40853 (7)	0.0706 (3)
N1	0.2654 (3)	0.8465 (2)	0.01587 (15)	0.0377 (5)
N2	0.1917 (6)	0.6486 (4)	0.5453 (2)	0.0788 (9)
O1	0.1170 (3)	0.9013 (2)	−0.15323 (16)	0.0571 (5)
O2	0.4735 (3)	0.8695 (2)	−0.17635 (15)	0.0565 (5)
O3	0.2242 (2)	0.68105 (19)	0.17640 (12)	0.0368 (4)
S1	0.28529 (9)	0.82249 (7)	−0.11866 (5)	0.03810 (19)
S2	0.33857 (15)	0.66455 (12)	0.42339 (7)	0.0734 (3)

have high toxicity to animals [8], and have adverse effects such as resistance to bacteria [9]. The compound dichlobentiazox described in this paper belongs to benzothiazole fungicides [10, 11], which show good plant disease control activity in plants without chemical damage.

In the molecules of the title structure bond lengths and angles are very similar to those given in the literature for benzo[*d*]isothiazole 1,1-dioxide [12–14]. In the title structure, the atoms of isothiazole ring and benzo[*d*]isothiazole 1,1-dioxide ring are approximately planar, and the dihedral angle between the isothiazole ring and the C1–C6 phenyl ring is 73°. The torsion angles of C6–C7–O3–C8 and C7–O3–C8–C9 are –178° and 176°, respectively.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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