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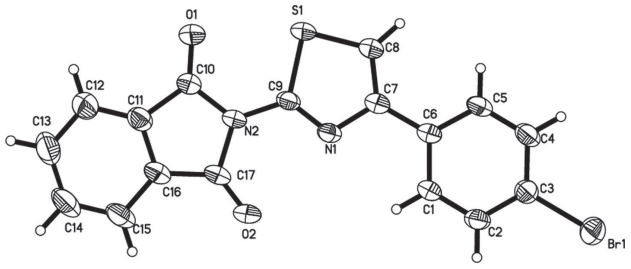
Crystal structure of 2-(4-(4-bromophenyl)thiazol-2-yl)isoindoline-1,3-dione, $C_{17}H_9BrN_2O_2S$



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Abstract

$C_{17}H_9BrN_2O_2S$, monoclinic, $P2_1/c$ (no. 14), $a = 11.2908(2)$ Å, $b = 8.3281(2)$ Å, $c = 16.1037(3)$ Å, $\beta = 94.453(1)°$, $V = 1509.67(5)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0348$, $wR_{ref}(F^2) = 0.1204$, $T = 296$ K.

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Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

4-(4-Bromophenyl)thiazol-2-amine (0.01 mol) were triturated and mixed with phthalic anhydride (1.48 g, 0.01 mol). The mixture was heated with occasional stirring for 2 h. The crude product was dissolved in hot EtOAc and filtered to remove any undissolved particles, and the 2-(4-(4-bromophenyl)thiazol-2-yl)isoindoline-1,3-dione was precipitated by cooling. The resulting precipitate was crystallized from ethanol to give crystals. Mp: 186–188°; yield: 82% [1].

Table 1: Data collection and handling.

Crystal:	Yellow, block, size 0.05×0.16×0.40 mm
Wavelength:	Cu K_α radiation (1.54178 Å)
μ:	51.03 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω scans
$2\theta_{max}$:	139.8°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	10104, 2809
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2577
$N(param)_{refined}$:	212
Programs:	Bruker programs [7], SHELX [8]

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

Atom	Site	x	y	z	U_{iso}
H(1A)	4e	0.1322	−0.1545	0.5466	0.043
H(2A)	4e	0.3014	0.0002	0.5495	0.045
H(4A)	4e	0.2407	0.0824	0.3044	0.050
H(5A)	4e	0.0712	−0.0707	0.3015	0.049
H(12A)	4e	−0.4852	−0.7383	0.6060	0.063
H(13A)	4e	−0.4826	−0.8160	0.7452	0.075
H(14A)	4e	−0.3288	−0.7377	0.8397	0.071
H(15A)	4e	−0.1758	−0.5788	0.7988	0.062
H(8)	4e	−0.086(4)	−0.241(6)	0.300(3)	0.09(1)

Experimental details

Cell refinement and data reduction were carried out by Bruker SAINT [7]. The hydrogen atoms were placed on calculated positions with the help of the SHELX program (AFIX 43 option) [8].

Discussion

The combination between thiazoles and phthalimides was founded in many biologically active compounds, which may act anticonvulsant, anticancer, antimicrobial, anti-inflammatory and antifungal [1–6]. In proceeds of our work, we report the crystal structure of the title compound ($C_{17}H_9BrN_2O_2S$). In the crystal structure the phenyl ring (C1—C6) and isoindoline-1,3-dione ring (N2/C10—C17) form

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Table 3: Fractional coordinates and atomic displacement parameters (Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1)	4*e*	0.42712(2)	0.18105(3)	0.42873(2)	0.0381(2)	0.0563(2)	0.0514(2)	−0.0079(1)	0.0020(1)	0.0068(1)
S(1)	4*e*	−0.21243(6)	−0.38848(9)	0.38389(3)	0.0515(4)	0.0669(4)	0.0225(3)	−0.0200(3)	−0.0100(2)	0.0034(2)
O(1)	4*e*	−0.3603(2)	−0.5734(2)	0.4711(1)	0.0467(9)	0.058(1)	0.0310(8)	−0.0135(8)	−0.0069(7)	−0.0005(7)
O(2)	4*e*	−0.0676(2)	−0.3978(2)	0.6641(1)	0.053(1)	0.065(1)	0.0257(7)	−0.013(1)	−0.0098(7)	0.0003(7)
N(1)	4*e*	−0.0519(2)	−0.3016(2)	0.4968(1)	0.035(1)	0.040(1)	0.0238(8)	0.0000(8)	−0.0030(7)	0.0010(7)
N(2)	4*e*	−0.1989(2)	−0.4664(2)	0.5496(1)	0.0377(9)	0.0430(9)	0.0208(8)	−0.0027(8)	−0.0044(7)	0.0004(7)
C(1)	4*e*	0.1540(2)	−0.1072(3)	0.4978(1)	0.041(1)	0.042(1)	0.0230(9)	−0.002(1)	−0.0016(8)	0.0031(8)
C(2)	4*e*	0.2552(2)	−0.0149(3)	0.4997(1)	0.038(1)	0.047(1)	0.026(1)	0.000(1)	−0.0030(8)	−0.0008(9)
C(3)	4*e*	0.2876(2)	0.0551(3)	0.4271(1)	0.032(1)	0.040(1)	0.034(1)	−0.0005(9)	0.0024(8)	0.0020(9)
C(4)	4*e*	0.2186(2)	0.0343(3)	0.3530(1)	0.044(1)	0.054(1)	0.027(1)	−0.000(1)	0.0017(9)	0.0087(9)
C(5)	4*e*	0.1175(2)	−0.0575(3)	0.3513(1)	0.043(1)	0.054(1)	0.024(1)	−0.002(1)	−0.0045(8)	0.0055(9)
C(6)	4*e*	0.0833(2)	−0.1312(3)	0.4235(1)	0.034(1)	0.038(1)	0.0231(9)	0.0036(9)	−0.0022(8)	0.0002(8)
C(7)	4*e*	−0.0236(2)	−0.2325(3)	0.4230(1)	0.036(1)	0.038(1)	0.026(1)	0.004(1)	−0.0020(8)	0.0007(8)
C(8)	4*e*	−0.0993(3)	−0.2664(4)	0.3561(1)	0.050(1)	0.057(1)	0.024(1)	−0.015(1)	−0.0049(9)	0.002(1)
C(9)	4*e*	−0.1473(2)	−0.3845(3)	0.4853(1)	0.037(1)	0.037(1)	0.0216(9)	−0.000(1)	−0.0035(8)	0.0011(8)
C(10)	4*e*	−0.3049(2)	−0.5549(3)	0.5377(1)	0.039(1)	0.042(1)	0.027(1)	−0.003(1)	0.0000(8)	−0.0017(9)
C(11)	4*e*	−0.3311(2)	−0.6153(3)	0.6208(1)	0.048(1)	0.041(1)	0.029(1)	−0.002(1)	0.0048(9)	−0.0023(9)
C(12)	4*e*	−0.4235(3)	−0.7075(4)	0.6443(2)	0.057(2)	0.062(2)	0.039(1)	−0.013(1)	0.008(1)	−0.004(1)
C(13)	4*e*	−0.4215(3)	−0.7530(4)	0.7274(2)	0.076(2)	0.067(2)	0.047(2)	−0.021(2)	0.024(1)	−0.001(1)
C(14)	4*e*	−0.3287(4)	−0.7052(4)	0.7845(2)	0.088(2)	0.062(2)	0.029(1)	−0.007(2)	0.015(1)	0.002(1)
C(15)	4*e*	−0.2372(3)	−0.6111(3)	0.7607(2)	0.072(2)	0.058(2)	0.025(1)	−0.001(2)	0.002(1)	0.002(1)
C(16)	4*e*	−0.2398(2)	−0.5660(3)	0.6777(1)	0.050(1)	0.043(1)	0.025(1)	0.002(1)	0.0010(9)	−0.0017(9)
C(17)	4*e*	−0.1547(2)	−0.4666(3)	0.6354(1)	0.045(1)	0.041(1)	0.0203(9)	0.004(1)	−0.0025(8)	−0.0013(8)

0.60(2)° and 1.96(3)° dihedral angles, respectively, with the central thiazole ring (C7/N1/C8/S1/C9), which make the whole molecule nearly planar (figure). In the crystal structure, molecules are at least linked by one non-classical hydrogen bond between C8—H8$\cdots$O2^{i} with the symmetry code: i = x, $-y-1/2$, $z-1/2$.

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