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N-(2-Bromothiazol-5-ylmethyl)phthalimide

Jiang-Tao Li, Jing-Kang Wang* and Li-Na Zhou

School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail: hangtohua@163.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.022
wR factor = 0.061
Data-to-parameter ratio = 13.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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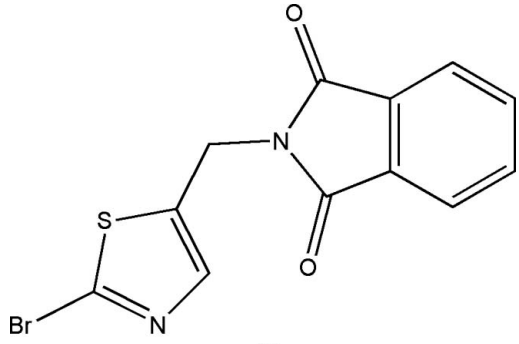
The title compound, $C_{12}H_7BrN_2O_2S$, is an very important intermediate in the synthesis of thiazole compounds. In the structure of the title compound, the phthalimide ring system and the thiazole ring are both planar, and the dihedral angle is 120°.

Comment

In recent years, thiazole compounds have become especially noteworthy. The thiazole ring has been incorporated into many different type of chemical structures, generating by structure modification a series of compounds with broad-spectrum bioactivities. Thus, thiazole compounds have played an increasingly important role in the production of highly active pesticides (Maienfisch *et al.*, 2001). 5-(Aminomethyl)-2-bromothiazole (II) is a very important intermediate in the synthesis of thiazole compounds. *N*-(2-Bromothiazol-5-ylmethyl)phthalimide, (I), a key intermediate in the synthesis of (II), is obtained by reaction of 2-bromo-5-(bromomethyl)-thiazole, dry DMF and potassium phthalimide. We report here the crystal structure of (I) (Fig. 1).



(I)

The title compound has two five-membered rings and a six-membered ring. As a result of the lack of hydrogen-bond donors, no inter- or intramolecular hydrogen bonds were observed.

Experimental

The synthesis of (I) was carried out according to (Uneme & Hideki, 1990). Potassium phthalimide (1.38 g) was added portionwise to a mixture of 2-bromo-5-(bromomethyl)thiazole (2.26 g) and dry DMF (35 ml) at room temperature, followed by stirring for an hour. The resulting insoluble substance was removed by filtration, the filtrate was concentrated and the residue purified by recrystallization from methanol, affording colorless crystals of (I).

Crystal data

$C_{12}H_7BrN_2O_2S$
M_r = 323.17
Triclinic, $P\overline{1}$
a = 7.3539 (15) Å
b = 8.6315 (17) Å
c = 9.794 (2) Å
α = 108.16 (3)°
β = 93.79 (3)°
γ = 96.41 (3)°
V = 583.7 (2) Å^3
Z = 2
D_x = 1.839 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.69 mm^{-1}
T = 293 (2) K
Block, colorless
0.57 × 0.56 × 0.53 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
φ ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.227, T_{max} = 0.244
(expected range = 0.131–0.141)
4808 measured reflections
2149 independent reflections
2047 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.061
S = 0.93
2149 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 0.2605P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.011
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

H atoms were positoned geometrically (C—H = 0.93–0.97 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; 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*.

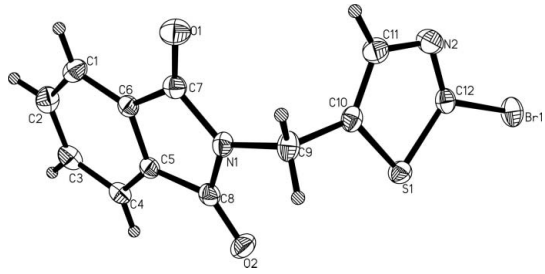


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

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