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2-(4-Amino-3-iodophenyl)-1,3-benzothiazole

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.006 Å
R factor = 0.030
wR factor = 0.072
Data-to-parameter ratio = 14.3

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

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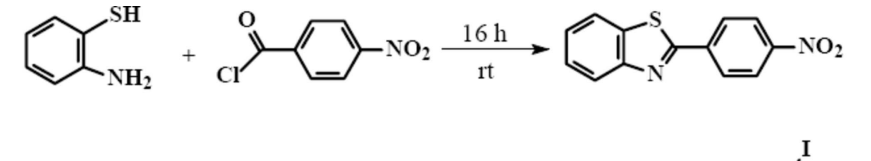
The title molecule, $C_{13}H_9IN_2S$, is composed of two planar units, namely a substituted aminophenyl ring and a benzothiazole ring system. The maximum deviations from the mean planes fitted through the ring atoms are only 0.010 (5) and 0.027 (6) Å for the aminophenyl and benzothiazole, respectively. In the solid state, the I atom lies on the same side of the molecule as the S atom rather than the N atom of the thiazole ring.

Comment

Alzheimer's disease (AD), the most common form of dementia in adults, is a neurodegenerative disease characterized by progressive cognitive decline, memory impairment and behavioural changes. Both the incidence and the prevalence of AD increase sharply with age. The accumulation of β-amyloid (Aβ) plaques in the brain may be a key risk factor associated with AD (Hardy *et al.*, 2002; Selkoe, 2000). Therefore, radiolabelled imaging probes for Aβ plaques may provide valuable information pertinent to the initiation and progression of AD. Of the Aβ-imaging agents that have been reported previously, radionuclide-labelled 2-(4-aminophenyl)benzothiazole (BTA) analogues are very promising. ^{123}I-labelled 2-(4-aminophenyl)benzothiazole is a potential Aβ imaging probe (Wang *et al.*, 2003). In order to study the quantitative structure–activity relationship of 2-(4-amino-3-iodophenyl)benzothiazole analogues, the determinaton of the structure of the title compound, (I), is important.



(I)

Iodination reactions may occur at the 3′- or 5′-position of 2-(4′-aminophenyl)benzothiazole. In order to confirm the position of the iodine, the structure of (I) was determined by a single-crystal X-ray diffraction experiment. The molecular structure of (I) is depicted in Fig. 1, and Fig. 2 shows a view of the unit cell contents. The ring atoms involved in both moieties are approxmately planar, with a maximum deviation of 0.060 (6) Å (Petricek *et al.*, 2006). In the solid state, the I atom lies on the same side of the molecule as the S atom rather than the N atom of the thiazole ring.

Table 1 lists some important bond distances, while Table 2 gives details of the hydrogen-bond interactions.

Experimental

The synthesis of (I) is shown in the scheme. The intermediate, 2-(4-aminophenyl)benzothiazole, was synthesized as described in the literature (Mathis *et al.*, 2002) and (I) was obtained as described by Shi *et al.* (1996). Suitable crystals were obtained by evaporation of an ethanol solution at room temperature for 7 d (m.p. 422–423 K).

Crystal data

$C_{13}H_9IN_2S$
M_r = 352.18
Monoclinic, $P2_1/c$
a = 7.8023 (3) Å
b = 8.7783 (4) Å
c = 18.5532 (10) Å
β = 97.446 (4)°
V = 1260.01 (10) Å^3
Z = 4
D_x = 1.857 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.69 mm^{-1}
T = 296 (2) K
Prism, colourless
0.30 × 0.13 × 0.09 mm

Data collection

Bruker SMART APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.658, T_{max} = 0.785
4249 measured reflections
2199 independent reflections
1552 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.072
S = 0.97
2199 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected bond lengths (Å).

I1—C2	2.100 (4)	S1—C7	1.752 (4)
S1—C8	1.735 (5)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···I1	0.86	2.79	3.248 (4)	115
N2—H2A···N1^{i}	0.86	2.26	3.097 (5)	166
C3—H3···S1	0.93	2.70	3.116 (4)	108

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

All H atoms were discernible in a difference Fourier map. They were placed in calculated positions (N—H = 0.86, C—H = 0.93) and refined using a riding model, U_{iso}(H) = 1.2U_{eq}(N,C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

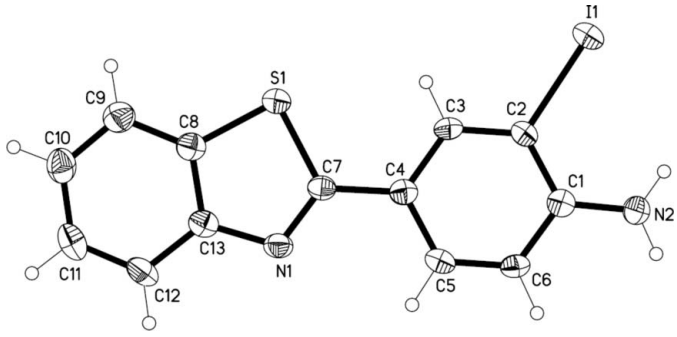


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level.

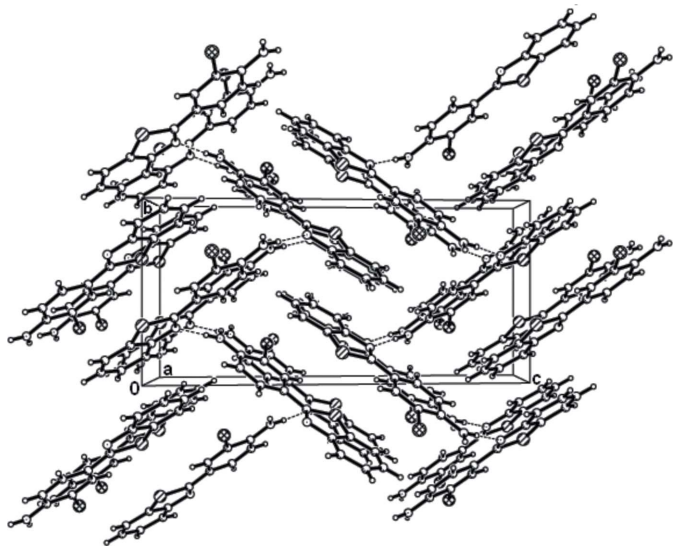


Figure 2
A packing diagram of (I). Dashed lines indicate hydrogen bonds.

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