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2-[4-(Dimethylamino)phenyl]-6-methoxy-1,3-benzothiazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.033
wR factor = 0.095
Data-to-parameter ratio = 13.1

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

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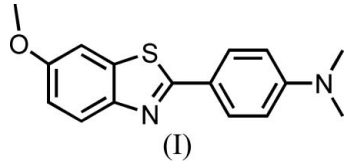
In the title compound, $C_{16}H_{16}N_2OS$, the benzothiazole ring system makes a dihedral angle of 8.64 (5)° with the dimethylaminophenyl group.

Comment

Benzothiazole aniline (BTA) analogues bind to β-amyloid plaques with high affinity (Klunk *et al.*, 2001). Their structures are very important for understanding the interaction between the ligand and the β-amyloid plaques. In the title compound, (I), Fig. 1, the benzothiazole ring system makes a dihedral angle of 8.64 (5)° with the dimethylaminophenyl group. Within the benzothiazole unit, the six-membered ring makes a dihedral angle of 2.29 (7)° with the five-membered ring.



(I)

Experimental

The title compound, (I), was prepared according to the literature procedure of Mathis *et al.* (2003). Single crystals suitable for X-ray diffraction studies were obtained by slow evaporation of a tetrahydrofuran solution over a period of two days.

Crystal data

$C_{16}H_{16}N_2OS$
M_r = 284.37
Monoclinic, $P2_1/n$
a = 14.997 (3) Å
b = 5.9717 (12) Å
c = 15.617 (3) Å
β = 101.24 (3)°
V = 1371.8 (5) Å^3
Z = 4
D_x = 1.377 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 293 (2) K
Prism, colorless
0.24 × 0.20 × 0.18 mm

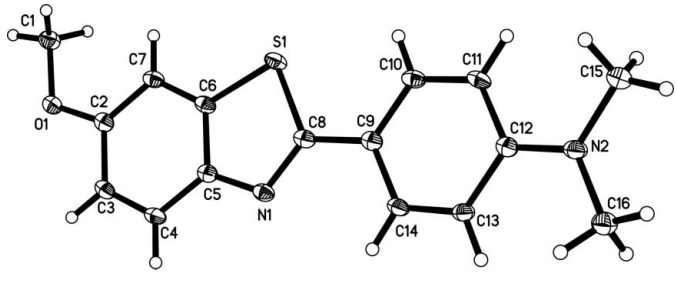


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level.

Data collection

Bruker P4 area-detector diffractometer	7871 measured reflections
ω scans	2405 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2153 reflections with $I > 2\sigma(I)$
$T_{min} = 0.946$, $T_{max} = 0.959$	$R_{int} = 0.025$
	$\theta_{max} = 25.0^{\circ}$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.283P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.033$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.095$	$\Delta\rho_{max} = 0.23$ e Å^{-3}
$S = 1.10$	$\Delta\rho_{min} = -0.24$ e Å^{-3}
2405 reflections	
184 parameters	
H-atom parameters constrained	

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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 1997); software used to prepare material for publication: *SHELXTL*.

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