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6-Bromo-1-methyl-4-[2-(4-methylbenzylidene)hydrazinylidene]-3*H*-2λ^6,1-benzothiazine-2,2-dione

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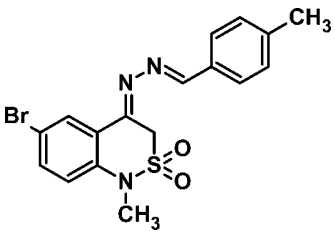
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.078; data-to-parameter ratio = 18.7.

In the title compound, $C_{17}H_{16}BrN_3O_2S$, the two fused rings are twisted by a dihedral angle of 6.61 (15)°. The thiazine ring adopts a sofa conformation. The toluene ring is oriented at dihedral angles of 15.5 (2) and 20.6 (2)° with respect to the bromobenzene and thiazine rings, respectively. The benzylidene system is approximately planar [r.m.s. deviation = 0.0388 Å]. In the cyrstal, weak intermolecular C—H···O hydrogen bonds connects the molecules into a chain along the b axis.

Related literature

For the synthesis of the title compound, see: Shafiq *et al.* (2011). For related structures, see: Khan *et al.* (2010); Shafiq *et al.* (2009); Arshad *et al.* (2009).



Experimental

Crystal data

$C_{17}H_{16}BrN_3O_2S$
M_r = 406.30
Monoclinic, $P2_1$
a = 9.1077 (6) Å
b = 6.8328 (4) Å
c = 14.1765 (9) Å
β = 96.807 (3)°
V = 876.00 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.48 mm^{-1}
T = 296 K
0.32 × 0.12 × 0.10 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.504, T_{max} = 0.790
10166 measured reflections
4119 independent reflections
2881 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.078
S = 0.97
4119 reflections
220 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983), 1771 Friedel pairs
Flack parameter: 0.004 (8)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17C···O1^{i}	0.96	2.64	3.546 (5)	158

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2429).

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