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N′-[(*E*)-1-(4-Bromophenyl)ethylidene]-4-hydroxy-2-methyl-1,1-dioxo-2*H*-1,2-benzothiazine-3-carbohydrazide

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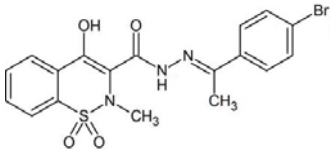
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.070; data-to-parameter ratio = 15.4.

The six-membered heterocycle in the title compound, $C_{18}H_{16}BrN_3O_4S$, adopts a sofa conformation. Intramolecular N—H···N and O—H···O hydrogen bonds stabilize the molecular conformation by forming a five- and a six-membered ring, respectively. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds.

Related literature

For general background, see: Zia-ur-Rehman *et al.* (2009). For synthesis details, see: Ahmad *et al.* (2011). For graph-set notation of hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{18}H_{16}BrN_3O_4S$
M_r = 450.31
Monoclinic, $P2_1/c$
a = 14.692 (2) Å
b = 16.562 (2) Å
c = 7.5254 (10) Å
β = 104.820 (1)°
V = 1770.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.47 mm^{-1}
T = 173 K
0.48 × 0.36 × 0.11 mm

Data collection

Siemens SMART diffractometer equipped with a Bruker KappaCCD APEXII
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.383, T_{max} = 0.773
21408 measured reflections
4490 independent reflections
3600 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.070
S = 1.03
4490 reflections
292 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17C···O2^{i}	0.95 (3)	2.38 (3)	3.275 (2)	158 (2)
C17—H17A···O4^{ii}	0.95 (3)	2.54 (3)	3.479 (2)	171 (2)
N2—H2N···N1	0.84 (3)	2.24 (3)	2.690 (2)	114 (2)
O1—H1O···O4	0.82 (3)	1.86 (3)	2.5979 (18)	148 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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 *X-SEED* (Barbour, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5633).

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