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6-Bromo-4-hydrazinylidene-1-methyl-3*H*-2λ^6,1-benzothiazine-2,2-dione

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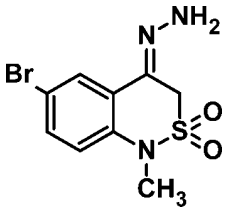
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.079; data-to-parameter ratio = 17.9.

In the title molecule, $C_9H_{10}BrN_3O_2S$, the thiazine ring has an envelope conformation with the S atom at the flap. The geometry around the S atom is distorted tetrahedral. In the crystal, inversion dimers linked by pairs of N—H···N hydrogen bonds occur, generating $R_2^2(6)$ ring motifs. N—H···O hydrogen bonds and C—H···O interactions connect the dimers, forming a three-dimentional network structure.

Related literature

For the related structures of 6-bromo-1-methyl-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide and 6-bromo-1-ethyl-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide, see: Shafiq *et al.* (2009*a*,*b*), respectively. For the structures of other benzothiazine derivatives, see: Shafiq *et al.* (2011); Arshad *et al.* (2011). For graph-set notation, see: Bernstein *et al.* (1995). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_9H_{10}BrN_3O_2S$
M_r = 304.17
Monoclinic, $P2_1/n$
a = 10.1483 (5) Å
b = 9.6375 (4) Å
c = 11.2118 (5) Å
β = 92.278 (2)°
V = 1095.69 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.93 mm^{-1}
T = 296 K
0.21 × 0.09 × 0.07 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.492, T_{max} = 0.771
12176 measured reflections
2719 independent reflections
1972 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.079
S = 1.01
2719 reflections
152 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H32···N2^{i}	0.85 (4)	2.47 (4)	3.198 (4)	144 (3)
N3—H31···O1^{ii}	0.90 (4)	2.38 (4)	3.252 (4)	162 (3)
C3—H3···O1^{iii}	0.93	2.45	3.323 (3)	156

Symmetry codes: (i) $-x+1, -y+2, -z+2$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

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: *ORTEP-3 for Windows* (Farrugia, 1997) and *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: SU2288).

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