6-Bromo-4-hydrazinylidene-1-methyl-3H-2λ6,1-benzothiazine-2,2-dione

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Key indicators: single-crystal X-ray study; T = 296 K; meanModelIndexer=[C–C] = 0.003 Å; R factor = 0.079; wR factor = 0.079; data-to-parameter ratio = 17.9.

In the title molecule, C9H10BrN3O2S, 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 R2(6) ring motifs. N—H···O hydrogen bonds and C—H···O interactions connect the dimers, forming a three-dimensional network structure.

Related literature

For the related structures of 6-bromo-1-methyl-1H-2,1-benzothiazin-4(3H)-one 2,2-dioxide and 6-bromo-1-ethyl-1H-2,1-benzothiazin-4(3H)-one 2,2-dioxide, see: Shafiq et al. (2009a,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).

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan
(SADABS; Bruker, 2001)
T min = 0.492, T max = 0.771
152 reflections with I > 2σ(I)

Refinement

R[F 2 > 2σ(F 2)] = 0.032
wR(F 2) = 0.079
S = 1.01
2719 reflections

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

Symmetry codes: (i) x+1, y, z; (ii) x, y+1, z; (iii) x−1, y−1, z+1.

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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).

References
