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# 4-Hydrazinylidene-1-methyl-3*H*-2$\lambda^6$,1-benzothiazine-2,2-dione

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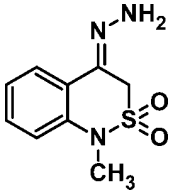
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.111; data-to-parameter ratio = 17.0.

In the title compound, $C_9H_{11}N_3O_2S$, the thiazine ring adopts a half-chair conformation. In the crystal structure N—H···N hydrogen bonds connect two molecules into a centrosymmetric dimer, forming an $R_2^2(6)$ ring motif. These dimers are further connected into chains by N—H···O and C—H···O hydrogen bonds.

## Related literature

For the synthesis of the title compound, see: Shafiq *et al.* (2011*b*). For information on 1,2 and 2,1-benzothiazine, see: Shafiq *et al.* (2011*a*); Arshad *et al.* (2011). For related structures, see: Tahir *et al.* (2008); Khan *et al.* (2010); Shafiq *et al.* (2009); Arshad *et al.* (2009). For graph-set notation of hydrogen bonds, see: Bernstein *et al.* (1995).



## Experimental

### Crystal data

$C_9H_{11}N_3O_2S$
$M_r$ = 225.27
Monoclinic, $P2_1/n$
$a$ = 6.6643 (2) Å
$b$ = 9.6834 (3) Å
$c$ = 15.5890 (5) Å
$\beta$ = 97.699 (1)°
$V$ = 996.94 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.31 mm$^{-1}$
$T$ = 296 K
0.41 × 0.22 × 0.18 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.884, $T_{max}$ = 0.947
8966 measured reflections
2426 independent reflections
2114 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.111
$S$ = 0.93
2426 reflections
143 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H1*N*···O1$^{i}$ | 0.86 (2) | 2.46 (2) | 3.221 (2) | 147.7 (17) |
| N3—H2*N*···N2$^{ii}$ | 0.790 (19) | 2.376 (19) | 3.094 (2) | 151.8 (19) |
| C8—H8*A*···O1$^{i}$ | 0.97 | 2.59 | 3.4178 (19) | 144 |

Symmetry codes: (i) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+3, -y, -z$.

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: *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: BT5565).

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