4-Hydrazinylidene-1-methyl-3H-2λ6,1-benzothiazine-2,2-dione

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Received 26 June 2011; accepted 9 July 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean ρ(C–C) = 0.002 Å;

For the synthesis of the title compound, see: Shafiq et al. (2011). For information on 1,2 and 2,1-benzothiazine, see: Shafiq et al. (2011a); 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).

In the title compound, C9H11N3O2S, the thiazine ring adopts a half-chair conformation. In the crystal structure N—H···O hydrogen bonds connect two molecules into a centrosymmetric dimer, forming an R2(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. (2011b). For information on 1,2 and 2,1-benzothiazine, see: Shafiq et al. (2011a); 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

C9H11N3O2S  b = 9.6834 (3) Å
M0 = 225.27
Monoclinic, P21/n
a = 6.6643 (2) Å
Z = 4

Mo Kα radiation
µ = 0.31 mm−1
T = 296 K
0.41 × 0.22 × 0.18 mm

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

D—H ⋅⋅⋅A  D—H  H ⋅⋅⋅A  D—A  D—H ⋅⋅⋅A
N3—H2i ⋅⋅⋅O1i  2.46 (2) 3.221 (2) 151.8 (19) 177.7 (17)
N3—H3i ⋅⋅⋅N2ii  2.876 (19) 3.094 (2) 151.8 (19) 167.7 (19)
C8—H8i ⋅⋅⋅O1i  2.59 3.218 (19) 143

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

The authors acknowledge the Higher Education Commission of Pakistan for providing a grant for the project to strengthen the Materials Chemistry Laboratory at GC University Lahore, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5565).

References