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2-Acetyl-4*H*-benzothiazin-3(2*H*)-one

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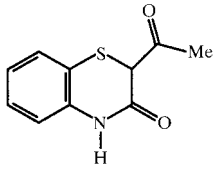
The title compound, $C_{10}H_9NO_2S$, has a boat-shaped heterocyclic six-membered ring such that the S and N atoms lie essentially in the plane of the benzene ring while the remaining two C atoms are above this plane.

Comment

4*H*-1,4-Benzothiazines have been reported to possess a wide spectrum of pharmacological properties similar to phenothiazines (Krapcho, 1976; Keyzer *et al.*, 1992; Chihara *et al.*, 1985; Corona *et al.*, 1992; Hiroyuki *et al.*, 1990). These products constitute an interesting series of heterocyclic compounds, not only from their biological activities, but also for structural investigations

The structure of the title compound, (I), was assigned on the basis of NMR and IR spectroscopy, and mass spectrometry, and by X-ray crystallography in order to establish its structure in the solid state. The S and N atoms of the six-membered heterocyclic ring lie almost in the plane of the benzene ring, such that the dihedral angle between the mean C_6 and SCCN planes is 176.4 (6)°. The other two C atoms of the heterocylic ring lie 0.4806 (3) and 1.0163 (3) Å above the SCCN mean plane. This corresponds to a boat conformation for the ring.



(I)

Experimental

Dithioaniline (10 g, 0.04 mol) was refluxed in a 250 ml two-necked round-bottomed flask equipped with a reflux condenser and a dropping funnel. Then ethyl acetoacetate (0.08 mol) in xylol (15 ml) was added dropwise. After 1.5 h the reaction was stopped, the solvent volume was reduced and the solution was allowed to settle. The product obtained was filtered off, washed with ether and recrystallized from ethanol (yield: 60%, m.p.: 447–449 K).

Crystal data

$C_{10}H_9NO_2S$	D_x = 1.448 Mg m^{-3}
M_r = 207.25	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6857 reflections
a = 11.384 (1) Å	θ = 1–26.4°
b = 10.202 (1) Å	μ = 0.31 mm^{-1}
c = 14.942 (2) Å	T = 298 K
β = 146.816 (6)°	Cube, colourless
V = 950.0 (9) Å^3	0.35 × 0.30 × 0.30 mm
Z = 4	

Data collection

KappaCCD diffractometer	R_{int} = 0.023
φ scans	θ_{max} = 26.38°
2011 measured reflections	$h = -14 \rightarrow 14$
1900 independent reflections	$k = -12 \rightarrow 0$
1741 reflections with $I > 3\sigma(I)$	$l = -18 \rightarrow 14$

Refinement

R = 0.032	H-atom parameters not refined
wR = 0.045	$w = 1/[\sigma^2(F_o^2) + 0.03F_o^2]$
S = 1.210	$(\Delta/\sigma)_{max}$ = 0.005
1741 reflections	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
127 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}

The difference Fourier maps showed that the methyl H atoms attached to the C14 atom have two equilibrium positions with an equal occupancy of 0.5.

Data collection: KappaCCD software; data reduction: *DENZO* and *SCALEPAK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *maXus* (Mackay *et al.*, 1999); software used to prepare material for publication: *maXus*.

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