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N-(2-Thiazol-2-yl)cyclopropanecarboxamide

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Key indicators

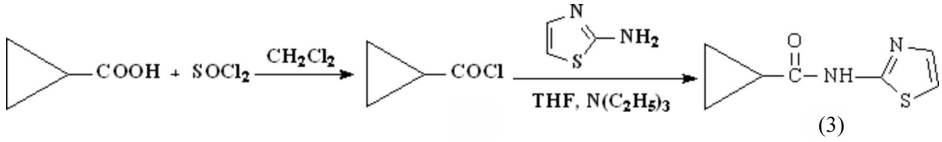
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.031
wR factor = 0.090
Data-to-parameter ratio = 14.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_7H_8N_2OS$, the thiazole ring makes a dihedral angle of 81.2 (3)° with the cyclopropane ring. The amide NH group and the thiazole N atom are linked by an intermolecular N—H···N hydrogen bond.

Comment

Cyclopropane derivatives have several biological activities. 1-Aminocyclopropane-1-carboxylic acid (ACC) is known to be the biochemical precursor of the plant hormone ethylene in a process catalysed by the ethylene-forming enzyme (EFE) (Adams *et al.*, 1979). 2,2-Dichloro-3,3-dimethylcyclopropanecarboxylic acid is an effective inducer against the rice blast fungus (Langcake *et al.*, 1983). A thiazole ring is often used as an active component in pesticide discovery. The title compound, (3), contains both active parts and may show some insecticidal activity. It was characterized by ^{1}H NMR and elemental analysis and its crystal structure is reported here.



(3)

The molecular structure of (3) is shown in Fig. 1. The dihedral angle between the thiazole and cyclopropane rings is 81.2 (3)°. The amide NH group and the thiazole N atom are linked by an intermolecular N—H···N hydrogen bond, forming dimers (Fig. 2 and Table 1).

Experimental

To a solution of cyclopropanecarboxylic acid (2 mmol, 0.17 g) in dichloromethane (10 ml) was added dropwise a solution of thionyl chloride (8 mmol, 0.6 ml) in dichloromethane (2 ml) at room temperature. The reaction mixture was kept at this temperature for

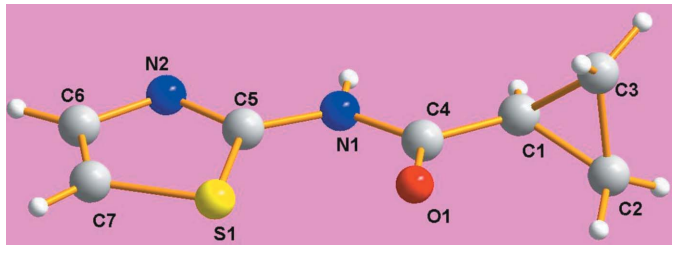


Figure 1
VThe molecular structure of (3), with displacement ellipsoids drawn at the 40% probability level.

1 h. The solution was concentrated to give cyclopropanecarbonyl chloride. 2-Aminothiazole (2 mmol, 0.19 g) and triethylamine (3 mmol, 0.4 ml) were dissolved in tetrahydrofuran (10 ml) with stirring, and cyclopropanecarbonyl chloride (0.21 g, 2 mmol) in tetrahydrofuran (5 ml) was added dropwise to the system at 273 K. The reaction mixture was kept at room temperature for 2–3 h, then filtered and concentrated. The residue was separated by silica-gel chromatography to afford the title compound, (3). Colourless single crystals were grown from a solution in AcOEt–cyclohexane (1:4). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41 (*d*, 1H, H6), 6.96 (*d*, 1H, H7), 1.80 (*m*, 1H, H1), 1.21 (*m*, 2H, H2), 0.98 (*m*, 2H, H3) Analysis calculated for $C_7H_8N_2O$ S: C 49.98, H 4.79, N 16.65%; found: C 50.01, H 4.78, N 16.68%.

Crystal data

$C_7H_8N_2OS$
M_r = 168.21
Monoclinic, $P2_1/c$
a = 5.707 (3) Å
b = 9.170 (4) Å
c = 15.453 (7) Å
β = 96.780 (5)°
V = 803.1 (6) Å^3
Z = 4
D_x = 1.391 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 294 (2) K
Block, colourless
0.24 × 0.22 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.919, T_{max} = 0.934
4114 measured reflections
1399 independent reflections
1215 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.090
S = 1.05
1399 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.049P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0045 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1′···N2^{i}	0.86	2.10	2.958 (2)	175

Symmetry code: (i) $-x, -y+1, -z$.

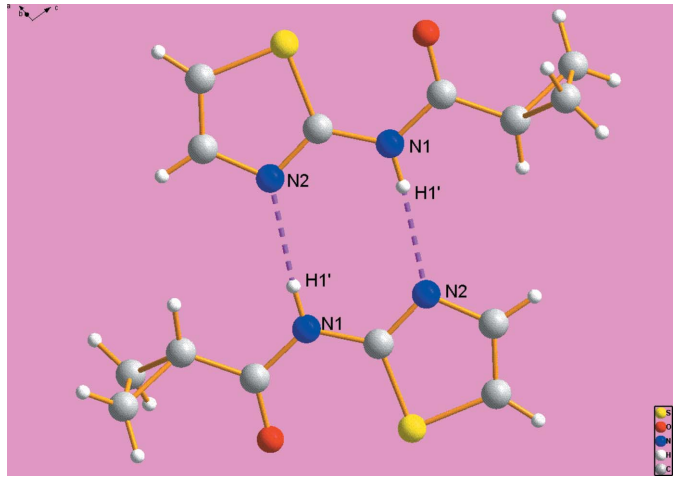


Figure 2
View of the hydrogen bonding (dashed lines) in (3). [Symmetry code: (i) $-x, -y+1, -z$.]

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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