Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-[3-(2-Chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarbonyl]thiazolidine-2-thione

Na-Bo Sun, De-Long Shen,* Jian-Quan Weng and Cheng-Xia Tan

College of Chemical Engineering and Materials Science, Zhejiang University of Technology, Hangzhou 310032, People's Republic of China

Correspondence e-mail: pesticide@zjut.edu.cn

Received 3 August 2006
Accepted 10 August 2006

The title compound, $C_{12}H_{13}ClF_3NOS_2$, was prepared by a condensation reaction of 3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarbonyl chloride and 1,3-thiazolidine-2-thione. In the crystal structure, the thiazolidine-2-thione group is in the thione form, although there may be tautomeric equilibrium with its thiol form in solution.

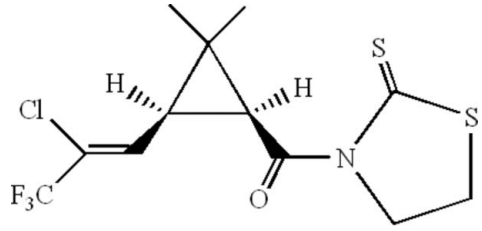
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.117
Data-to-parameter ratio = 19.3

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

Comment

Cycloprothrin derivatives have a high potential for biological activity. They are commonly characterized by low toxicity and good environmental compatibility. In addition, 1,3-thiazolidine-2-thione derivatives have been widely used in agrochemical fungicides because of their high biological activity (Takashi *et al.*, 1997). As part of our attempts to find new pesticides, we have synthesized the title compound, (I), and determined the structure. The thiazolidine-2-thione group of (I) is in the thione form (Fig. 1), although 1,3-thiazolidine-2-thione exists in tautomeric equilibrium with its thiol form in solution (Atzei *et al.*, 2001).



(I)

Experimental

1,3-Thiazolidine-2-thione (1.05 g, 8.8 mmol), prepared according to the procedure of Owen (1967), and triethylamine (1.20 g, 11.9 mmol) were dissolved in dichloromethane (15 ml) with stirring. 3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarbonyl chloride (2.60 g, 10 mmol) was added dropwise to the mixture at room temperature. The mixture was stirred at room temperature for 15 h and then dried *in vacuo* to give a yellow solid, compound (I) (yield: 2.24 g, 74.1%), which was then recrystallized from ethanol to give yellow needles (m.p. 408–410 K).

Crystal data

$C_{12}H_{13}ClF_3NOS_2$
M_r = 343.81
Monoclinic, $P2_1/c$
a = 14.667 (8) Å
b = 9.585 (4) Å
c = 11.774 (5) Å
β = 112.131 (18)°
V = 1533.2 (12) Å^3
Z = 4
D_x = 1.489 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.55 mm^{-1}
T = 298 (1) K
Thick needle, yellow
0.31 × 0.16 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.835, T_{max} = 0.926
14633 measured reflections
3513 independent reflections
2015 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.040
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.117
S = 1.02
3513 reflections
182 parameters
H-atom parameters constrained
$w = 4F_o^2/[0.0005F_o^2 + \sigma(F_o^2)]$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 21 (2)

H atoms were placed in calculated positions and refined using the riding-model approximation, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

The authors thank Mr Jianmin Gu for assistance in the data collection.

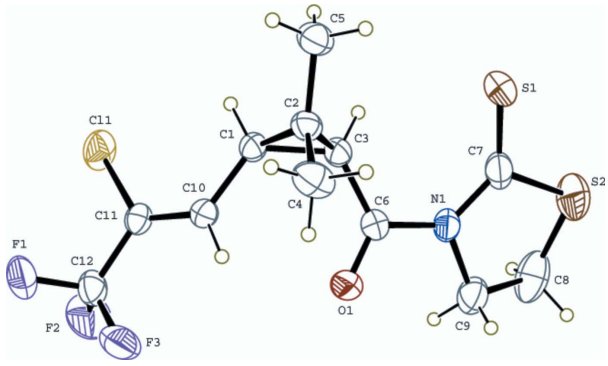


Figure 1
The molecular structure of (I), showing 40% probability displacement ellipsoids.

References

Atzei, D., Filippo, D. D., Rossi, A. & Porcelli, M. (2001). *Spectrosc. Acta A*, **57**, 1073–1083.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Larson, A. C. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 291–294. Copenhagen: Munksgaard.
Owen, T. C. (1967). *J. Chem. Soc.* **15**, 1373–1376.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2004). *CrystalStructure*. Version 3.7.0. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97*. University of Göttingen, Germany.
Takashi, J., Nakaya, M., Inami, S. & Matsuno, H. (1997). JP Patent No. 09,124,647.