Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-[(*E*)-2-Chloro-3,3,3-trifluoroprop-1-en-1-yl]-*N*-(2-chlorophenyl)-2,2-dimethylcyclopropane-1-carboxamide

Dong-Qing Liu,[a] Fan-Yong Yan,[b]* Yun-Ying Gao,[b] Lei Guo[b] and Zi Kong[b]

[a]School of Materials Science and Engineering, Tianjin Polytechnic University, Tianjin 300160, People's Republic of China, and [b]School of Materials and Chemical Engineering, Tianjin Polytechnic University, Tianjin 300160, People's Republic of China
Correspondence e-mail: yfany@yahoo.com

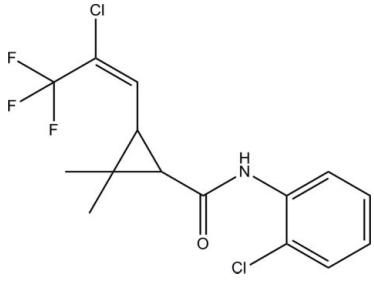
Received 16 November 2010; accepted 3 December 2010

Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.115; data-to-parameter ratio = 18.8.

In the title compound, $C_{15}H_{14}Cl_2F_3NO$, synthesized by the reaction of 3-[(*E*)-2-chloro-3,3,3-trifluoroprop-1-enyl]-2,2-dimethylcyclopropanecarboxylic acid and 2-chloroaniline, the aromatic ring makes a dihedral angle of 76.7 (3)° with the plane of the cyclopropane ring. In the crystal, intermolecular N—H···O hydrogen bonds link the molecules into chains running along the *b* axis.

Related literature

The title compound is an intermediate for tefluthrinn (2,3,5,6-tetrafluoro-4-methylbenzyl(1*RS*,3*RS*)-3-[(*Z*)-2-chloro-3,3,3-trifluoroprop-1-enyl]-2,2-dimethylcyclopropanecarboxylate), an insecticide controlling a wide range of soil insect pests, see: Punja (1981). For the preparation of the title compound, see Liu & Yan (2007). For a related structure, see: Yan *et al.* (2011).



Experimental

Crystal data

$C_{15}H_{14}Cl_2F_3NO$
M_r = 352.17
Orthorhombic, *Pbca*
a = 18.454 (4) Å
b = 9.3350 (19) Å
c = 18.981 (4) Å
V = 3269.7 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.43 mm^{-1}
T = 113 K
0.40 × 0.06 × 0.06 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.848, T_{max} = 0.975
28276 measured reflections
3873 independent reflections
3325 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.115
S = 1.08
3873 reflections
206 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.81 (2)	2.26 (2)	3.0415 (19)	162 (2)

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation (No. 20376059) and Tianjin Polytechnic University

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5407).

References

Liu, D.-Q. & Yan, F.-Y. (2007). *Acta Cryst.* E**63**, o4202.
Punja, N. (1981). Eur. Patent EP 0031199.
Rigaku/MSC (2005). *CrystalClear*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yan, F. Y., Liu, D.-Q., Wen, J.-Y., Gao, Y.-Y. & Li, A.-M. (2011). *Acta Cryst.* E**67**, o60.