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3-[2,2-Dichloro-1-(4-ethoxyphenyl)cyclopropanecarbonyl]oxazolidin-2-one

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The title compound, $C_{15}H_{15}Cl_2NO_4$, a cyclopropane derivative related to the insecticide cycloprothrin, was prepared from oxazolidin-2-one and 2,2-dichloro-1-(4-ethoxyphenyl)cyclopropanecarbonyl chloride. The five-membered oxazolidine ring is planar to within 0.045 Å; the cyclopropane ring plane forms approximately equal dihedral angles with the mean planes of the oxazolidine and benzene rings [62.7 (4) and 61.6 (4)°, respectively].

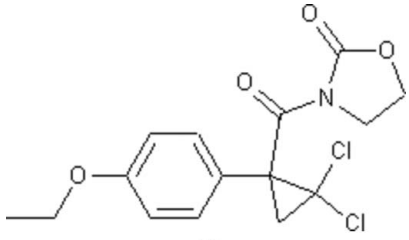
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.100
Data-to-parameter ratio = 17.9

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. These derivatives have been widely used in the manufacture of pesticides (Holan *et al.*, 1986). As part of our ongoing studies of the structure–activity relationships for cycloprothrin derivatives and related compounds, we have isolated the title compound, (I), using the reaction of oxazolidin-2-one and 2,2-dichloro-1-(4-ethoxyphenyl)cyclopropanecarbonyl chloride.



(I)

The molecular structure of (I) is shown in Fig. 1. The oxazolidine ring (N1/C5/C6/O2/C7) is planar to within 0.045 Å; the cyclopropane ring (C1–C3) forms dihedral angles of 62.7 (4) and 61.6 (5)° with the least-squares planes of the oxazolidine and benzene (C8–C13) rings, respectively. The orientation of the carbonyl group relative to the cyclopropane ring may be described by the torsion angle *X*1—C1—C4—O1 of 91.9°, where *X*1 is the centroid of the cyclopropane ring.

Experimental

Oxazolidin-2-one (0.70 g, 8 mmol) and triethylamine (1.11 g, 11 mmol) were dissolved in dichloromethane (15 ml) with stirring, and 2,2-dichloro-1-(4-ethoxyphenyl)cyclopropanecarbonyl chloride (2.94 g, 10 mmol) was added dropwise to the mixture at room temperature. The mixture was then stirred at 303 K for 10 h, washed three times with water and dried, yielding 2.36 g of a solid product (yield 68.5%). This was recrystallized from ethanol and gave colourless blocks (m.p. 428–430 K) suitable for an X-ray study.

Crystal data

$C_{15}H_{15}Cl_2NO_4$
M_r = 344.19
Monoclinic, $P2_1/c$
a = 10.131 (4) Å
b = 15.345 (8) Å
c = 10.505 (4) Å
β = 105.846 (16)°
V = 1571.1 (12) Å^3
Z = 4
D_x = 1.455 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.43 mm^{-1}
T = 296 (1) K
Block, colourless
0.42 × 0.36 × 0.30 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.822, T_{max} = 0.879
16981 measured reflections
3579 independent reflections
2113 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.100
S = 1.00
3579 reflections
200 parameters
H-atom parameters constrained
$w = 1/[0.77\sigma(F_o^2)]/(4F_o^2)$
$(\Delta/\sigma)_{max}$ <0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

H atoms were included in calculated positions (C—H = 0.96 Å for methyl, 0.93 Å for aromatic, and 0.97 Å for the remaining H atoms) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(parent atom) (1.5U_{eq} for methyl H atoms).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1993); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

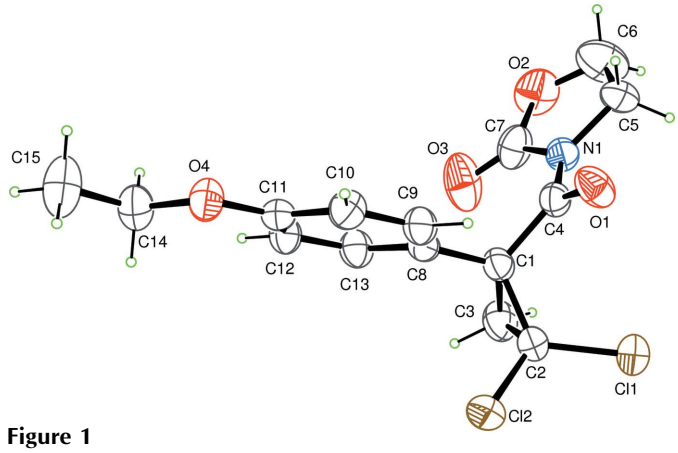


Figure 1
The molecular structure of (I), showing the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level.

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