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3-(2,4-Dichloro-5-isopropyloxyphenyl)-5-*tert*-butyl-1,3,4-oxadiazol-2-one

Guo-Lin Zhang

Department of Medicinal Chemistry, College of Pharmaceutical Science, Zhejiang University, Hangzhou 310031, People's Republic of China

Correspondence e-mail: guolinzhang@zju.edu.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.087
Data-to-parameter ratio = 20.2

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

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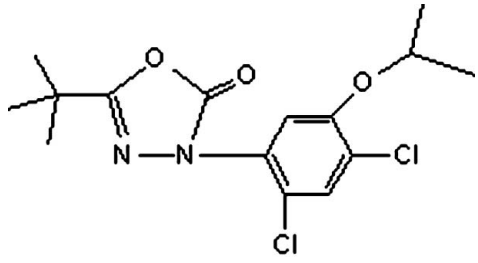
The title compound, $C_{15}H_{18}Cl_2N_2O_3$, is an effective herbicide. The oxadiazolone ring is not coplanar with the benzene ring. Pairs of molecules form centrosymmetric dimers *via* weak C—H···O hydrogen bonds.

Comment

1,3,4-Oxadiazole derivatives exhibit many biological activities, for example antibacterial (Maslat *et al.*, 2002), antifungal (Dubey & Sangwan, 1994) and anti-inflammatory activities (Omar *et al.*, 1996). The title compound, (I) (oxadiazon) is an effective herbicide for controlling weeds and increasing seed yield in soya beans (Dubey *et al.*, 1988).



(I)

The structure determination of (I) was carried out in order to determine its molecular conformation. The torsion angles of the atoms in the oxadiazolone ring show that this ring is almost planar. The C7—N1—C1—C2 torsion angle of −65.8 (2)° shows that oxadiazolone ring is not coplanar with the benzene ring.

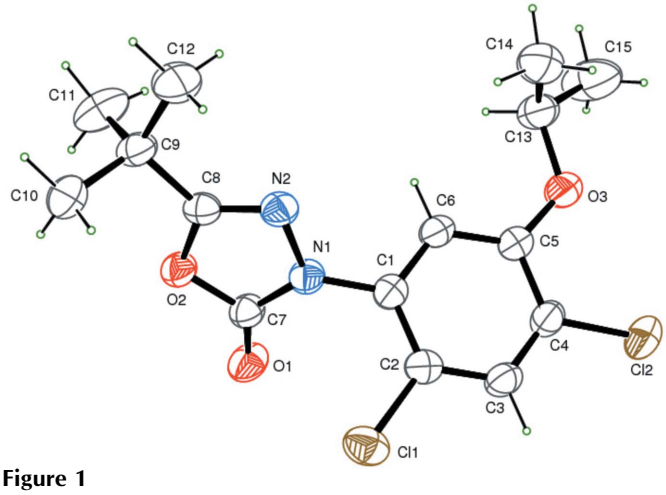


Figure 1
A view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 40% probability level.

Pairs of molecules form centrosymmetric dimers *via* weak C—H···O hydrogen bonds (Fig. 2).

Experimental

A solution of 1-trimethylacetyl-2-(2,4-dichloro-5-isopropyloxyphenyl)hydriazine (20 mmol) in toluene (20 ml) and a 20% solution of carbonyl chloride in toluene (30 ml) were mixed and heated gradually to about 373–383 K, until the evolution of gas ceased. The reaction mixture was then cooled to room temperature. After concentration of the toluene solution under reduced pressure, the residual solid was recrystallized from ethanol to give the title compound. Diffraction quality crystals of (I) were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{15}H_{18}Cl_2N_2O_3$
M_r = 345.22
Monoclinic, $P2_1/c$
a = 9.700 (4) Å
b = 11.068 (4) Å
c = 16.514 (8) Å
β = 94.135 (19)°
V = 1768.2 (13) Å^3
Z = 4
D_x = 1.297 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 298 (1) K
Platelet, colourless
0.47 × 0.40 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.830, T_{max} = 0.927
16776 measured reflections
4042 independent reflections
2237 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.033
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.087
S = 1.01
4042 reflections
200 parameters
H-atom parameters constrained
$w = 1/[0.0002F_o^2 + 1.1\sigma(F_o^2)]/(4F_o^2)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 6.8 (3) × 10^2

All H atoms were placed in geometrically idealized positions, with C—H distances ranging from 0.93 to 0.98 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

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.*, 1999); 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*.

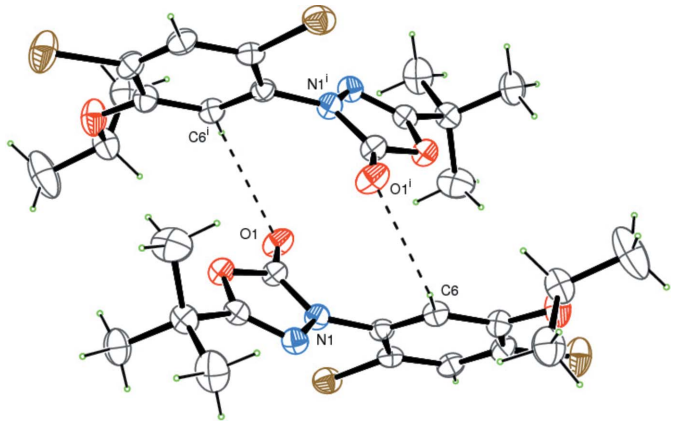


Figure 2
A view of two molecules connected by C—H···O hydrogen bonds (dashed lines) [Symmetry code: (i) 2 − x, 1 − y, 1 − z.]

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