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5-Chloromethyl-3-(2,4-dichlorophenyl)-1,2,4-oxadiazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.150
Data-to-parameter ratio = 15.1

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

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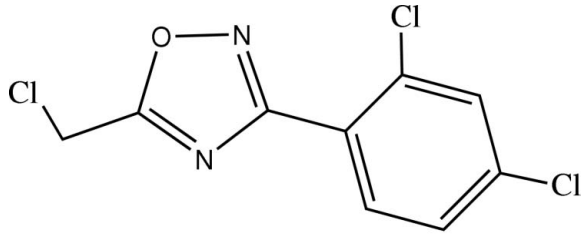
In the title compound, $C_9H_5Cl_3N_2O$, the dihedral angle between the oxadiazole and benzene rings is 9.0 (2)°. There are intra- and intermolecular C—H···N interactions in the crystal structure.

Comment

Some derivatives of 1,2,4-oxadiazoles have intrinsic analgesic (Terashita *et al.*, 2002), anti-inflammatory (Nicolaides *et al.*, 1998) and antipicornaviral (Romero, 2001) properties and are efficient as agonists [*e.g.* for angiotensin (Naka *et al.*, 1999) and adhesion (Juraszyk *et al.*, 1997)] for different receptors.



(I)

We report here the crystal structure of the title compound, (I). The plane of the oxadiazole ring makes a dihedral angle of 9.0 (2)° with the C4–C9 benzene ring (Fig. 1). There are intra- and intermolecular C—H···N interactions in the crystal structure (Table 1).

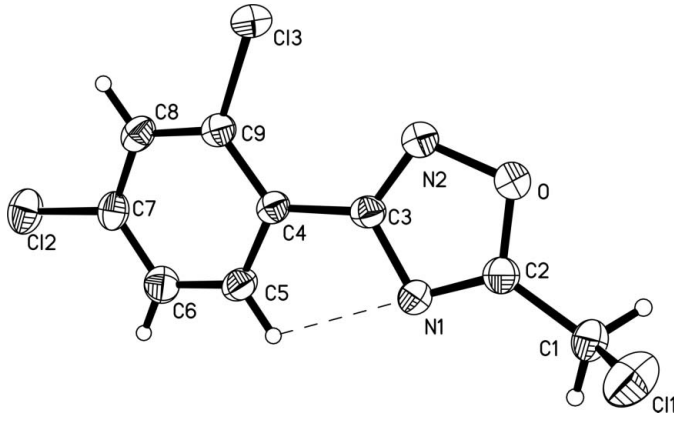


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level. The dashed line indicates a C—H···N interaction.

Experimental

A solution of chloracetyl chloride (14 mmol) in toluene (10 ml) was added dropwise to a solution of 2,4-dichlorobenzamidoxime (14 mmol) in toluene (60 ml). The resulting mixture was refluxed for 6 h. After cooling and filtration, crude compound (I) was obtained. It was purified by recrystallization from a mixture of ethyl acetate (15 ml) and petrolum ether (7.5 ml) (yield 75.2%). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_9H_5Cl_3N_2O$
$M_r = 263.50$
Monoclinic, $P2_1/n$
$a = 7.9010\ (16)$ Å
$b = 14.987\ (3)$ Å
$c = 9.7400\ (19)$ Å
$\beta = 113.20\ (3)^\circ$
$V = 1060.1\ (4)$ Å^3
$Z = 4$
$D_x = 1.651$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.84$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.40 × 0.40 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.731$, $T_{max} = 0.788$
2218 measured reflections
2068 independent reflections
1624 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 26.0^\circ$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.150$
$S = 1.05$
2068 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.062 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···N2^{i}	0.97	2.51	3.468 (4)	171
C5—H5A···N1	0.93	2.45	2.825 (4)	104

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

All H atoms were positioned geometrically and refined in a riding-model approximation, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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