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5-[1-(3,4-Dichlorophenoxy)ethyl]-1,3,4-oxadiazole-2(3H)-thione hemihydrate

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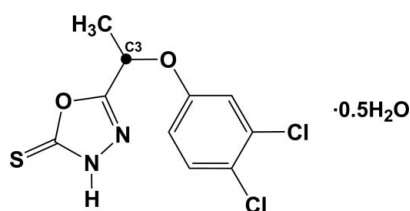
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 Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.027; wR factor = 0.078; data-to-parameter ratio = 19.1.

In the title compound, $\text{C}_{10}\text{H}_8\text{Cl}_2\text{N}_2\text{O}_2\text{S}\cdot 0.5\text{H}_2\text{O}$, the atoms in the oxadiazole ring are essentially coplanar (r.m.s. deviation 0.010 Å). The crystal structure is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds involving the water molecule, which is situated on an a twofold rotation axis, and two organic molecules, leading to a thione tautomer in the solid state. The C atom attached to the oxadiazole ring adopts a typical sp^3 hybridization. The dihedral angle between the mean plane of the benzene ring of the dichlorophenyl group and the mean plane of the oxadiazole ring is $74.18(4)^\circ$. The crystal structure is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{S}$ hydrogen bonds.

Related literature

For the structures and properties of oxadiazoles, see: Almasirad *et al.*, (2004); Aboraia *et al.* (2006); Akhtar, Hameed, Al-Masoudi *et al.* (2008); Khan *et al.* (2005); Akhtar, Hameed *et al.* (2007); Akhtar, Hameed, Khan *et al.* (2008); Akhtar, Rauf *et al.* (2007); Aydogan *et al.*, (2002). For a related structure, see: Thamotharan *et al.* (2005). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{10}\text{H}_8\text{Cl}_2\text{N}_2\text{O}_2\text{S}\cdot 0.5\text{H}_2\text{O}$
 $M_r = 300.15$
 Monoclinic, $C2/c$
 $a = 11.8725(2)$ Å
 $b = 7.89320(10)$ Å
 $c = 26.6092(4)$ Å
 $\beta = 92.9130(10)^\circ$

$V = 2490.38(6)$ Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.68$ mm⁻¹
 $T = 123$ K
 $0.40 \times 0.30 \times 0.25$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: none
 10568 measured reflections

3088 independent reflections
 2490 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.078$
 $S = 1.09$
 3088 reflections
 162 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1W}$	0.86	2.06	2.9084 (16)	168
$\text{O1W}-\text{H1W}\cdots\text{S1}^i$	0.846 (17)	2.612 (18)	3.3854 (13)	152.5 (17)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2129).

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