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[2-(4-Chlorophenyl)-1,3-selenazol-4-yl]-methanol

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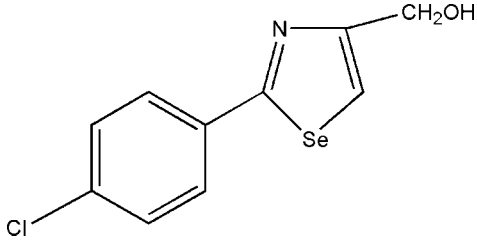
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.041; wR factor = 0.104; data-to-parameter ratio = 13.6.

In the title compound, $C_{10}H_8ClNOSe$, the dihedral angle between benzene and selenazole rings is 11.4 (3)° and the hydroxymethyl group is bent from the selenazole ring, making a dihedral angle of 63.8 (3)°. In the crystal, molecules are linked into inversion dimers by pairs of O—H···N hydrogen bonds. Roof-tile-like stacking of the molecules along [010] [b = 4.5707 (4) Å] is observed, with the benzene and selenazole rings separated by a face-to-face distance of 3.57 Å and a mutual slippage of 2.85 Å.

Related literature

For the synthesis of 1,3-selenazoles and their biological activity, see: Shafiee *et al.* (1979); Koketsu & Ishihara (2003); Geisler *et al.* (2004). For crystal structures of 1,3-selenazole derivatives, see: Shen *et al.* (2011); Shi & Zhao, (2007).



Experimental

Crystal data

$C_{10}H_8ClNOSe$ M_r = 272.58
Monoclinic, $P2_1/c$
a = 14.8150 (15) Å
b = 4.5707 (4) Å
c = 14.9123 (14) Å
β = 96.642 (1)°
V = 1003.01 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.97 mm^{-1}
T = 298 K
0.35 × 0.32 × 0.15 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.337, T_{max} = 0.587
4466 measured reflections
1742 independent reflections
1318 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.104
S = 1.01
1742 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	2.07	2.891 (5)	174

Symmetry code: (i) $-x+1, -y, -z+1$.

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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QK2047).

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Shi, X. & Zhao, G.-L. (2007). *Acta Cryst.* E**63**, o3642.

supporting information

Acta Cryst. (2012). E**68**, o3458 [doi:10.1107/S1600536812048088]

[2-(4-Chlorophenyl)-1,3-selenazol-4-yl]methanol

Jichun Cui, Chuan Li and Yanling Qiao

S1. Comment

It has well been confirmed that selenium-containing heterocyclic compounds are of considerable biochemical and pharmacological relevance. Thus, derivatives of selenazole have been extensively studied not only because of their interesting reactivities but also because of their pharmaceutical applications (Koketsu & Ishihara, 2003; Geisler *et al.*, 2004). Interested in this field, the title compound, a derivative of selenazole, was prepared and its crystal structure presented (Fig. 1). In the title compound, $C_{10}H_8NOClSe$, the dihedral angle between the nearly planar benzene and selenazole rings is 11.4 (3)°. The dihedral angle between the selenazole ring and the hydroxymethyl group, defined by C9—C10–O1, is 63.8 (3)°. All the bond lengths and angles are normal and correspond to those observed in the related compounds (Shen *et al.*, 2011; Shi & Zhao, 2007). In the crystal structure, pairs of molecules are disposed about an inversion center, generating dimers linked by intermolecular O—H···N hydrogen bonds (Fig. 2 and Table 1). The aromatic parts of the molecules are stacked along [010] (b = 4.5707 (4) Å) in a roof tile-like fashion enabling slipped π-π-stacking interactions. The face-to-face distance of the aromatic parts of the molecules (Se1, N1, C1 – C9) is 3.57 Å and their slippage 2.85 Å approximately parallel to the ring-to-ring bond C4—C7 (Fig. 2). This brings Cl1 in a position above/below the ring centroid of an adjacent benzene ring (Cl···centroid (C1 – C6) = 3.68 Å).

S2. Experimental

2-(4-Chlorophenyl)-4-chloromethyl-1,3-selenazole (0.01 mol) (Shafiee *et al.*, 1979) was added to dilute sulfuric acid (75 ml, 3.5 mol L^{-1}) and heated at reflux for 8 h. The solution was made alkaline with dilute sodium hydroxide and extracted with chloroform. The organic layer was dried with Na_2SO_4, filtered, and evaporated and the obtained solid was recrystallized from ethanol. Clear block-shaped crystals were obtained.

S3. Refinement

C-bonded H atoms were placed in calculated positions and thereafter treated as riding, C—H = 0.93 and 0.97 Å, U_{iso}(H) = 1.2U_{eq}(C). The hydroxyl H atom was refined with AFIX 147 of program *SHELXL97* (Sheldrick, 2008), O—H = 0.82 Å, U_{iso}(H) = 1.5U_{eq}(O).

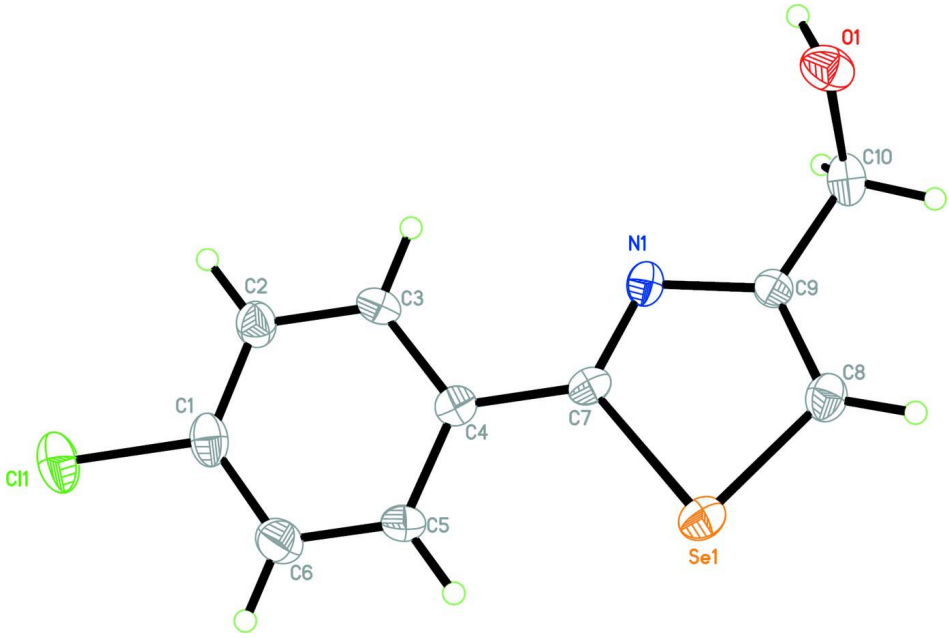

Figure 1

The molecular structure of the title compound with 50% probability displacement ellipsoids.

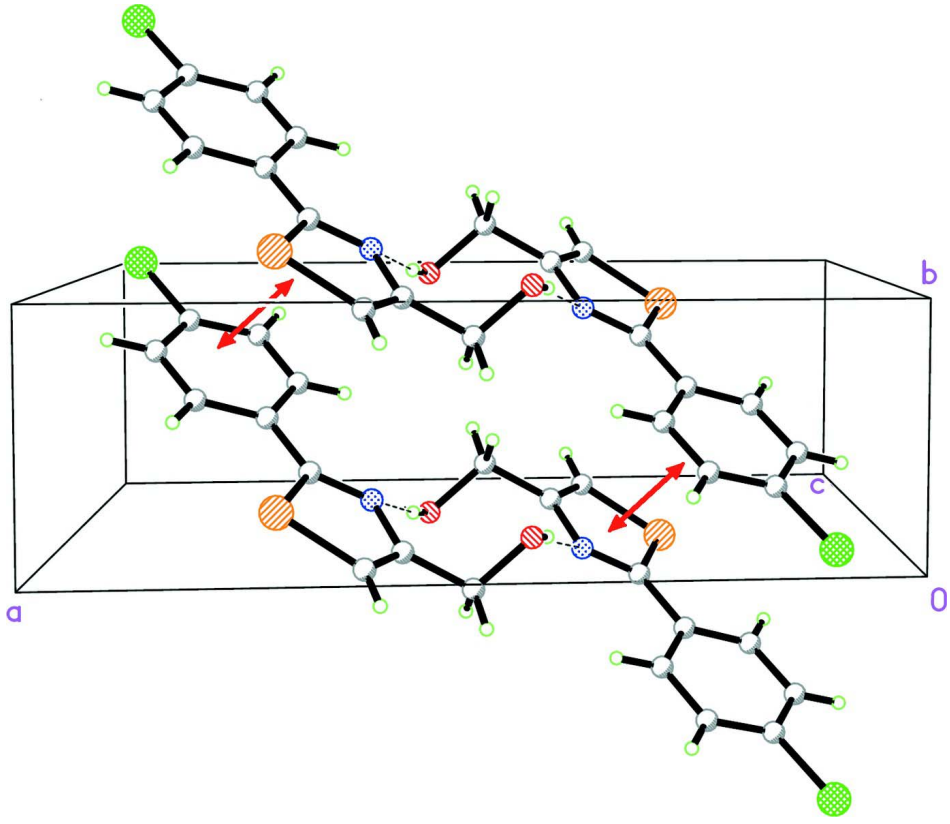

Figure 2

Packing diagram of the title compound indicating H-bonds by dashed lines and π-π-stacking by red double arrows (see Table 1 and text).

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Crystal data

$C_{10}H_8ClNOSe$
$M_r = 272.58$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.8150\ (15)$ Å
$b = 4.5707\ (4)$ Å
$c = 14.9123\ (14)$ Å
$\beta = 96.642\ (1)°$
$V = 1003.01\ (16)$ Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.805$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1928 reflections
$\theta = 2.8–27.1°$
$\mu = 3.97$ mm^{-1}
$T = 298$ K
Block, white
0.35 × 0.32 × 0.15 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
π and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.337$, $T_{max} = 0.587$
4466 measured reflections
1742 independent reflections
1318 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -15\rightarrow17$
$k = -5\rightarrow5$
$l = -17\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.104$
$S = 1.01$
1742 reflections
128 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Se1	0.74166 (3)	0.13939 (10)	0.30636 (3)	0.0423 (2)
Cl1	0.93843 (9)	1.0498 (3)	0.66855 (9)	0.0586 (4)
O1	0.4348 (2)	−0.0090 (8)	0.3910 (2)	0.0465 (8)
H1	0.4149	−0.0297	0.4396	0.070*
N1	0.6330 (2)	0.1313 (7)	0.4388 (2)	0.0313 (8)
C1	0.8698 (3)	0.8234 (9)	0.5942 (3)	0.0394 (11)
C2	0.7838 (3)	0.7563 (10)	0.6124 (3)	0.0401 (11)
H2	0.7612	0.8350	0.6628	0.048*
C3	0.7307 (3)	0.5702 (9)	0.5551 (3)	0.0352 (10)
H3	0.6722	0.5232	0.5672	0.042*
C4	0.7644 (3)	0.4523 (9)	0.4790 (2)	0.0308 (10)
C5	0.8507 (3)	0.5313 (11)	0.4624 (3)	0.0410 (11)
H5	0.8735	0.4589	0.4112	0.049*

C6	0.9042 (4)	0.7147 (11)	0.5196 (3)	0.0503 (13)
H6	0.9626	0.7637	0.5078	0.060*
C7	0.7083 (3)	0.2511 (9)	0.4200 (2)	0.0285 (9)
C8	0.6372 (3)	−0.0813 (9)	0.2973 (3)	0.0373 (11)
H8	0.6171	−0.1989	0.2481	0.045*
C9	0.5933 (3)	−0.0506 (9)	0.3712 (2)	0.0293 (9)
C10	0.5071 (3)	−0.2087 (10)	0.3850 (3)	0.0410 (11)
H10A	0.4912	−0.3417	0.3349	0.049*
H10B	0.5167	−0.3236	0.4399	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.0457 (4)	0.0490 (4)	0.0337 (3)	−0.0017 (2)	0.0118 (2)	−0.0033 (2)
Cl1	0.0543 (9)	0.0538 (9)	0.0629 (8)	−0.0135 (6)	−0.0131 (6)	−0.0081 (6)
O1	0.037 (2)	0.060 (2)	0.0427 (18)	0.0018 (18)	0.0058 (15)	0.0102 (16)
N1	0.034 (2)	0.029 (2)	0.0299 (17)	0.0012 (16)	−0.0013 (15)	−0.0014 (14)
C1	0.042 (3)	0.031 (3)	0.042 (2)	−0.002 (2)	−0.008 (2)	0.0014 (19)
C2	0.049 (3)	0.037 (3)	0.034 (2)	−0.008 (2)	0.005 (2)	−0.0008 (19)
C3	0.027 (3)	0.041 (3)	0.039 (2)	−0.004 (2)	0.0053 (19)	0.0034 (19)
C4	0.035 (3)	0.029 (2)	0.028 (2)	0.0021 (19)	0.0035 (18)	0.0047 (16)
C5	0.027 (3)	0.046 (3)	0.052 (3)	−0.002 (2)	0.013 (2)	−0.009 (2)
C6	0.036 (3)	0.047 (3)	0.069 (3)	−0.004 (2)	0.010 (3)	−0.005 (3)
C7	0.030 (3)	0.029 (2)	0.0265 (19)	0.0094 (19)	0.0022 (17)	0.0039 (17)
C8	0.040 (3)	0.039 (3)	0.032 (2)	0.004 (2)	−0.0018 (19)	−0.0006 (18)
C9	0.027 (2)	0.029 (2)	0.030 (2)	0.0053 (18)	−0.0034 (18)	0.0012 (17)
C10	0.042 (3)	0.039 (3)	0.039 (2)	−0.007 (2)	−0.004 (2)	−0.002 (2)

Geometric parameters (Å, º)

Se1—C8	1.839 (5)	C3—H3	0.9300
Se1—C7	1.889 (4)	C4—C5	1.378 (6)
Cl1—C1	1.753 (4)	C4—C7	1.463 (6)
O1—C10	1.419 (6)	C5—C6	1.380 (6)
O1—H1	0.8200	C5—H5	0.9300
N1—C7	1.303 (5)	C6—H6	0.9300
N1—C9	1.383 (5)	C8—C9	1.350 (6)
C1—C2	1.367 (6)	C8—H8	0.9300
C1—C6	1.370 (6)	C9—C10	1.502 (6)
C2—C3	1.385 (6)	C10—H10A	0.9700
C2—H2	0.9300	C10—H10B	0.9700
C3—C4	1.399 (5)		
C8—Se1—C7	84.78 (19)	C1—C6—C5	118.8 (5)
C10—O1—H1	109.5	C1—C6—H6	120.6
C7—N1—C9	113.5 (4)	C5—C6—H6	120.6
C2—C1—C6	121.5 (4)	N1—C7—C4	125.2 (4)
C2—C1—Cl1	119.6 (4)	N1—C7—Se1	113.5 (3)

C6—C1—Cl1	118.9 (4)	C4—C7—Se1	121.3 (3)
C1—C2—C3	119.5 (4)	C9—C8—Se1	111.3 (3)
C1—C2—H2	120.3	C9—C8—H8	124.3
C3—C2—H2	120.3	Se1—C8—H8	124.3
C2—C3—C4	120.4 (4)	C8—C9—N1	116.9 (4)
C2—C3—H3	119.8	C8—C9—C10	123.9 (4)
C4—C3—H3	119.8	N1—C9—C10	119.1 (4)
C5—C4—C3	118.1 (4)	O1—C10—C9	111.1 (4)
C5—C4—C7	122.0 (4)	O1—C10—H10A	109.4
C3—C4—C7	119.9 (4)	C9—C10—H10A	109.4
C6—C5—C4	121.8 (4)	O1—C10—H10B	109.4
C6—C5—H5	119.1	C9—C10—H10B	109.4
C4—C5—H5	119.1	H10A—C10—H10B	108.0
C6—C1—C2—C3	1.1 (7)	C3—C4—C7—N1	−11.4 (6)
Cl1—C1—C2—C3	−178.0 (3)	C5—C4—C7—Se1	−11.1 (6)
C1—C2—C3—C4	−0.2 (7)	C3—C4—C7—Se1	169.0 (3)
C2—C3—C4—C5	−1.1 (6)	C8—Se1—C7—N1	0.0 (3)
C2—C3—C4—C7	178.7 (4)	C8—Se1—C7—C4	179.7 (3)
C3—C4—C5—C6	1.7 (7)	C7—Se1—C8—C9	0.3 (3)
C7—C4—C5—C6	−178.2 (5)	Se1—C8—C9—N1	−0.6 (5)
C2—C1—C6—C5	−0.6 (7)	Se1—C8—C9—C10	−178.4 (3)
Cl1—C1—C6—C5	178.5 (4)	C7—N1—C9—C8	0.6 (5)
C4—C5—C6—C1	−0.8 (7)	C7—N1—C9—C10	178.6 (4)
C9—N1—C7—C4	−180.0 (4)	C8—C9—C10—O1	−117.4 (4)
C9—N1—C7—Se1	−0.3 (4)	N1—C9—C10—O1	64.8 (5)
C5—C4—C7—N1	168.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	2.07	2.891 (5)	174

Symmetry code: (i) −*x*+1, −*y*, −*z*+1.